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| (54) Title: METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR COACTIVATOR BINDING | | |
| (57) Abstract <p>The present invention relates to methods and agonist/antagonist compounds for modulating nuclear receptor coactivator binding. The invention includes a method for identifying residues comprising a coactivator binding site for a nuclear receptor of interest. Also included is a method of identifying agonists and/or antagonists that bind to a coactivator binding site of a nuclear receptor of interest. Agonists and antagonists of coactivator binding to nuclear receptors also are provided. The invention is exemplified by identification and manipulation of the coactivator binding site of the thyroid receptor (TR), and compounds that bind to these sites. The methods can be applied to other nuclear receptors including RAR, RXR, PPAR, VDR, ER, GR, PR, MR, and AR.</p> | | |

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METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR COACTIVATOR BINDING

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INTRODUCTION

Technical Field

The present invention relates to methods and compounds for modulating nuclear receptor coactivator binding.

Background

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Cells contain receptors that can elicit a biological response by binding various molecules including proteins, hormones and/or drugs. Nuclear receptors represent a super family of proteins that are hormone/ligand-activated transcription factors that enhance or repress transcription in a cell type-, ligand- and promoter-dependent manner. The nuclear receptor family includes receptors for glucocorticoids (GRs), androgens (ARs), mineralocorticoids (MRs), progestins (PRs), estrogens (ERs), thyroid hormones (TRs), vitamin D (VDRs), retinoids (RARs and RXRs), peroxisomes (XPARs and PPARs) and icosanoids (IRs). The so-called "orphan receptors" for which ligands have not been identified are also part of the nuclear receptor superfamily, as they are structurally homologous to the classic nuclear receptors, such as steroid and thyroid receptors.

5 Although overall sequence conservation between nuclear receptors varies between different families of receptors, sequence conservation between functional regions, or modules, of the receptors is high. For example, nuclear receptors can be organized into functional modules comprising an N-terminal transcriptional activation domain, a central DNA binding domain (DBD), and a C-terminal ligand binding domain (LBD). The LBD of nuclear receptors represents a hormone/ligand-
10 dependent molecular switch. Binding of hormone to a nuclear receptor's LBD changes its ability to modulate transcription of DNA, although they may have transcription-independent actions. Nuclear receptors also bind proteins, such as chaperone complexes, corepressors, or coactivators, that are involved in receptor function. Hormone binding by a nuclear receptor can increase or decrease binding affinity to these proteins, and can influence or mediate the multiple actions of the nuclear
15 receptors on transcription. For example, nuclear receptors can stimulate transcription in response to hormone binding by recruiting coactivator proteins to promoters of responsive genes (Glass et al., *Curr. Opin. Cell Biol.* (1997) 9:222-32); and Horwitz et al., *Mol. Endocrinol.* (1996) 10:1167-77).

Coactivators of the p160 family mediate activity of a transcriptional activation domain, called AF2, that is part of the nuclear receptor's LBD. A few receptor mutants deficient in
20 coactivator-dependent activation have been isolated (TR: Collingwood et al. *Proc. Natl. Acad. Sci.* (1997) 94:248-253; VDR: Jurutka et al., *J. Biol. Chem.* (1997) 272:14592-14599, Masayama et al., *Mol. Endocrinol.* (1997) 11:1507-1517; ER and RAR: Henttu et al., *Mol. Cell Biol.* (1997) 17:1832-1839). While these studies support the physiological relevance of the observed interaction, the structural and functional nature of the site to which coactivators bind has not been defined.

25 The medical importance of nuclear receptors is significant. They have been implicated in breast cancer, prostate cancer, cardiac arrhythmia, infertility, osteoporosis, hyperthyroidism, hypercholesterolemia, obesity and other conditions. However, limited treatments are available and current agonist/antagonist drugs used to target nuclear receptors are ligands that bind to the receptor's LBD buried deep within the receptor. Although additional targets on nuclear receptors
30 are desired for drug development, the structural and functional basis of such sites, including the coactivator binding site, has not been described.

Accordingly, a need exists for identification and characterization of the coactivator binding sites of nuclear receptors, and molecules that affect their interaction with cellular coactivator proteins. This would provide a major new target for iterative drug design, synthesis, and selection.
35 It also would be advantageous to devise methods and compositions for reducing the time required to discover compounds that target the coactivator binding site of nuclear receptors and administer them to organisms to modulate physiological processes regulated by nuclear receptors.

5 **Relevant Literature**

Wagner et al., (*Nature* (1995) 378:690-697) disclose the crystal structure of rat TR-alpha LBD. Various references disclose mutations in carboxyl-terminal helices of nuclear receptors (Henttu et al., *supra*; O'Donnell et al., *Mol. Endocrinol.* (1991) 5:94-99; Whitfield et al., *Mol. Endocrinol.* (1995) 9:1166-79; Saatcioglu et al., *Mol. Cell Biol.* (1997) 17:4687-95; Collingwood et al., *supra*; Kamei et al., *Cell* (1996) 85:403-14). Hong et al. (*Proc. Natl. Acad. Sci. USA* (1996) 93(10):498-49452) and Hong et al. (*Mol. Cell. Biol.* (1997) 17:2735-2744) disclose cloning and expression of GRIP1 coactivator. Torchia et al., (*Nature* (1997) 387:677-84), Le Douarin et al., (*EMBO J* (1996) 15:6701-6715) and Heery et al. (*Nature* (1997) 387:733-736) disclose sequence alignment of various coactivator proteins showing a (SEQ ID NO: 1) LxxLL motif.

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SUMMARY OF THE INVENTION

The present invention relates to identification and manipulation of the coactivator binding site of nuclear receptors. Identification of this site permits design and obtention of compounds that bind to the coactivator binding site of nuclear receptors and modulate coactivator binding to the receptor. The compounds include agonists and antagonists that modulate nuclear receptor activity by promoting (agonists) or blocking (antagonists) hormone-dependent coactivator binding to the receptor, particularly antagonists. The compounds of the invention can be receptor-, cell- and/or tissue-specific.

The present invention also includes protein cocrystals of nuclear receptors with a molecule bound to the coactivator binding site and methods for making them. The cocrystals provide means to obtain atomic modeling information of the specific amino acids and their atoms forming the coactivator binding site and that interact with molecules that bind to the site, such as coactivator. The cocrystals also provide modeling information regarding the coactivator:nuclear receptor interaction, as well as the structure of coactivators bound thereto.

The present invention further provides methods for identifying and designing small molecules that bind to the coactivator binding site using atomic models of nuclear receptors. The method involves modeling test compounds that fit spacially into a nuclear receptor coactivator binding site of interest using an atomic structural model comprising a nuclear receptor coactivator binding site or portion thereof, screening the test compounds in a biological assay characterized by

- 5 binding of a test compound to a nuclear receptor coactivator binding site, and identifying a test compound that modulates coactivator binding to the nuclear receptor.

The invention also includes compositions and methods for identifying coactivator binding sites of nuclear receptors. The methods involve examining the surface of a nuclear receptor of interest to identify residues that modulate coactivator binding. The residues can be identified by
10 homology to the coactivator binding site of human TR described herein. Overlays and superpositioning with a three dimensional model of a nuclear receptor LBD, or a portion thereof that contains a coactivator binding site, also can be used for this purpose. Additionally, alignment and/or modeling can be used as a guide for the placement of mutations on the LBD surface to characterize the nature of the site in the context of a cell.

- 15 Also provided is a method of modulating the activity of a nuclear receptor. The method can be *in vitro* or *in vivo*. The method comprises administering, *in vitro* or *in vivo*, a sufficient amount of a compound that binds to the coactivator binding site. Preferred compounds bind to the site with greater affinity than coactivator proteins found in a cell of interest. Binding at this site, the compound can compete for binding of coactivator proteins, thereby inhibiting gene transcription, or
20 in some cases promoting it, even when hormone is or is not bound.

The invention further includes a method for identifying an agonist or antagonist of coactivator binding to a nuclear receptor. The method comprises providing the atomic coordinates comprising a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system; modeling compounds which fit spacially into the nuclear receptor coactivator
25 binding site; and identifying in an assay for nuclear receptor activity a compound that increases or decreases activity of the nuclear receptor through binding the coactivator binding site.

Also provided is a machine-readable data storage medium with information for constructing and manipulating an atomic model comprising a coactivator binding site or portion thereof. The medium comprises a data storage material encoded with machine readable data which, when using a
30 machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex for a nuclear receptor coactivator binding site.

Also provided is a method of identifying a compound that selectively modulates the activity of one type of nuclear receptor compared to other nuclear receptors. The method is exemplified by
35 modeling test compounds that fit spacially and preferentially into a nuclear receptor coactivator

5 binding site of interest using an atomic structural model of a nuclear receptor coactivator binding site, selecting a compound that interacts with one or more residues of the coactivator binding site unique in the context of that site, and identifying in an assay for coactivator binding activity a compound that selectively binds to the coactivator binding site compared to other nuclear receptors. The unique features involved in receptor-selective coactivator binding can be identified by
10 comparing atomic models of different receptors or isoforms of the same type of receptor.

The invention finds use in the selection and characterization of peptide, peptidomimetic, as well as other small molecule compounds, such as small organic molecules, identified by the methods of the invention, particularly new lead compounds useful in treating nuclear receptor-based disorders.

15

BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1 shows the specific effects of mutations on hTR β 1 transcriptional activation in HeLa cells and correlation with effects on binding to GST-GRIP1. T₃ dependent activation of transcription of a reporter gene, expressed as the percentage of WT is plotted for each mutant.
20 GST-GRIP1 binding, analyzed by autoradiography after separation using 10% SDS-PAGE, was also expressed as the percentage of WT and plotted for each mutant. The GST-GRIP1 used included GRIP1 amino acids 721-1121; the same results were obtained using a GST-GRIP1 construct including GRIP1 amino acids 563-1121 (data not shown).

Figure 2 shows that overexpression of full-length GRIP1 rescues loss of transcriptional
25 activation by hTR β 1 mutants. Indicated amounts of the expression vector for full-length GRIP1; pSG5-GRIP1, is included in the cotransfections, which otherwise are performed as in **Figure 1**. The WT or different representative hTR β 1 mutants are indicated.

Figure 3 shows specific hER α surface mutants cause loss of transcriptional activation in HeLa cells in parallel with their loss of *in vitro* GRIP1 binding. The fold E₂ activation, expressed as
30 the percentage of WT, and the phosphorimager quantitation of *in vitro* binding of [³⁵S]-labeled hER α WT and mutants to GST-GRIP1 (GRIP1 amino acids 721-1121) also expressed as the percentage of WT is plotted for each mutant.

5 **Figure 4** shows a plot of the fold E_2 activation observed when the indicated amounts of the full-length GRIP1 expression vector, pSG5-GRIP1, are added to the co-transfection experiment, which otherwise is performed as for **Figure 3**. The WT or different hER α mutants are indicated. The data represent the averages of three independent experiments, with standard deviations less than 10%.

10 **Figure 5** shows a CPK model of the TR α -LBD, indicating the LBD surface locations of mutations made in the full-length hTR β 1. Mutated residues having no effect on GRIP1 binding or effect on activation in HeLa cells are shaded gray. Mutated residues with diminished GRIP1 and SRC-1 α binding and diminished activation in HeLa cells are colored to reflect chemical properties of the residues: red, blue (purple), and green indicate acidic, basic, and hydrophobic residues,
15 respectively. The main chain structures of the TR α - and TR β -LBDs are the same (data not shown).

Figure 6 shows sequence alignment of amino acid residues of members of the p160 coactivator family. Single amino acid designations are used. Members of the p160 coactivator family interact with the nuclear receptors through conserved (SEQ ID NO: 1) LxxLL motifs.

Figure 7 shows binding affinity assays of GST-GRIP1 constructs with NR-boxes 1, 2,
20 and/or 3 and their interaction with TR LBD. GRIP-1 NR boxes 1,2 and 3 interact differently with TR β LBD. Single letter designations are used for the amino acids.

Figure 8 shows binding affinity assays of GST-GRIP1 constructs with NR-boxes 1, 2, and/or 3 and their interaction with TR and GR LBDs. TR and GR differ in their interactions with GRIP-1.

25 **Figure 9** shows binding affinity assays for NR-box 2- and 3-peptides and GRIP1 and their interaction with TR LBD. NR box 2- and 3-containing peptides reproduce the affinity and specificity of the NR interaction domain.

Figure 10 shows binding affinity assays for NR-box 2- and 3-peptides and their interaction with TR LBD. Sequence adjacent to the (SEQ ID NO: 1) LxxLL motif modulate the affinity of
30 NR-box-TR β LBD interactions.

5 **Figure 11** shows binding affinity assays for mutant GRIP1 and NR-box 2- and 3-peptides and their interaction with TR LBD. The individual leucine residues of the (SEQ ID NO: 1) LxxLL motif are crucial for binding of the GRIP-1 NR interaction domain to TR β LBD.

10 **Figure 12** shows the contents of the asymmetric unit of the crystallized hTR β LBD:GRIP1 NR-box 2 peptide complex. The crystal lattice consists of a repeating unit containing a 2:2 complex of hTR LBD and GRIP1 site 2 peptide. Positions of the two GRIP1 site 2 peptides are boxed, in green (site 1), and red (site 2), with the peptides drawn as a C-alpha trace. The two NCS related monomers of the hTR LBD are shown as a secondary structure ribbon drawing, with monomer 1 in light grey, and monomer 2 in dark grey. The side chains of the hydrophobic residues I689, L690, L693, L694 of the GRIP1 NR-box 2 peptides are drawn to emphasize those interactions observed in
15 both bound peptides.

Figure 13 shows a ribbon diagram depicting the interaction of the GRIP1 NR-box 2 peptide with the hTR β LBD. The GRIP1 NR-box 2 peptide (dark grey) forms three turns of α -helix, and binds the hTR LBD (light gray) in a hydrophobic cleft defined by helices H3, H4, H5, and H12. Portions of the hTR β LBD, and the neighboring monomer, are omitted for clarity.

20 **Figure 14** shows interface between the GRIP1 NR-box 2 peptide and the hTR β LBD. Side chains of residues of the hTR β LBD within 4.5Å of the GRIP-1 NR-box 2 peptide are labeled. The color of the individual side chains reflects the chemical nature of the residue: acidic residues are red, basic residue are blue, aliphatic residues are green, aromatic residues are brown, and polar residues are orange. The peptide is depicted as a C-alpha trace with the side chains of (SEQ ID
25 NO: 2) ILxxLL motif shown explicitly.

Figure 15 shows residues in the hTR β LBD that are necessary for transactivation. The transactivation mutations are mapped onto the interface between the GRIP1 NR-box 2 peptide and the hTR β LBD.

30 **Figure 16** shows molecular surface of the hTR LBD. The side chains of the leucines residues fit within a hydrophobic groove formed from helices H3, H5, and H12, while the side chain of the non-conserved isoleucine residue packs against the outside edge of the groove. The remainder of the peptide is shown as main chain.

5 **Figure 17** shows complementarity between the (SEQ ID NO: 1) LxxLL motif and the surface of the hTR LBD. The side chains of the (SEQ ID NO: 2) ILxxLL motif are shown in a CPK representation, with the main chain of the peptide drawn as a C-alpha trace. The three leucine residues fit into pockets of the coactivator binding site of the hTR β LBD, depicted as mesh, while the isoleucine residue rests on the edge of the site's cleft.

10 **Figure 18** shows the coactivator binding site cleft, one side of which is formed by conformationally hormone-responsive residues. On the left is a view of the TR-LBD molecular surface showing the concave surfaces in gray. The cavity is shown at the center of the figure. On the right is shown a CPK model of the TR-LBD, overlaid with a molecular surface view, which is restricted to a 12Å radius of the hydrophobic cavity. Mutated residues of the coactivator binding
15 site that are hormone-insensitive (V284, K288, I302 and K306) are located on one side of the cleft and are colored yellow. Mutated CBS residues likely undergo a conformational change upon hormone binding (L454 and E457) are located on the opposite side of the cleft and are colored red.

20 **Figure 19** shows alignment of amino acid sequences (single letter amino acid designations) containing residues that form the coactivator binding sites of several nuclear receptors. The boxes represent residues of alpha-helix (H3, H4, H5, H6 and H12); lower case letters "h" and "q" represent hydrophobic and polar residues, respectively.

5

DESCRIPTION OF SPECIFIC EMBODIMENTS

The present invention provides methods and compositions for identifying compounds that modulate nuclear receptor activity. The compounds can be nuclear receptor agonists or antagonists that bind to the coactivator binding site (and that act as mimetics to the coactivator in this regard), and promote (agonists) or block (antagonists) binding of the coactivator to the target nuclear receptor. Compounds that bind to the coactivator binding site also are provided. The compounds can be natural or synthetic. Preferred compounds are small organic molecules, peptides and peptidomimetics (e.g., cyclic peptides, peptide analogs, or constrained peptides).

As described in the Examples, mutagenesis and coactivator binding studies, coupled with analysis of atomic models derived from cocrystals, reveals for the first time a previously unknown structure for nuclear receptors, the coactivator binding site. By "coactivator binding site" is intended a structural segment or segments of nuclear receptor polypeptide chain folded in such a way so as to give the proper geometry and amino acid residue conformation for binding a coactivator. This is the physical arrangement of protein atoms in three-dimensional space forming a coactivator binding site pocket or cavity. Residues forming the site are amino acids corresponding to (i.e., the same as or equivalent to) human TR residues of C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Leu454, Glu457, Val458 and Phe459). The coactivator binding site is highly conserved among the nuclear receptor super family (Figure 19). Thus, this site corresponds to a surprisingly small cluster of residues on the surface of the LBD that form a prominent hydrophobic cleft. The hydrophobic cleft is formed by hydrophobic residues corresponding to human TR residues of C-terminal helix 3 (Ile280, Val283, Val284, and Ala287), helix 4 (Phe293), helix 5 (Ile302 and Leu305), helix 6 (Cys309), and helix 12 (Leu454, Val458 and Phe459). The hydrophobic cleft of the coactivator binding site also is highly conserved among the nuclear receptor super family (Figure 19).

The invention also includes compositions and methods for identifying coactivator binding sites of nuclear receptors. The methods involve examining the surface of a nuclear receptor of interest to identify residues that modulate coactivator binding. The residues can be identified by homology to the coactivator binding site of human TR described herein. A preferred method is alignment with the residues of any nuclear receptor corresponding to (i.e., equivalent to) human TR

5 residues of the C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459). Overlays and superpositioning with a three-dimensional model of a nuclear receptor LBD, or a portion thereof that contains a coactivator binding site, also can be used for this purpose. For example, three-dimensional structures of TR, RAR, RXR and ER
10 LBDs can be used for this purpose. For example, nuclear receptors identifiable by homology alignment include normal nuclear receptors or proteins structurally related to nuclear receptors found in humans, natural mutants of nuclear receptors found in humans, normal or mutant receptors found in animals, as well as non-mammalian organisms such as pests or infectious organisms, or viruses.

15 Alignment and/or modeling also can be used as a guide for the placement of mutations on the LBD surface to characterize the nature of the site in the context of a cell. Selected residues are mutated to preserve global receptor structure and solubility. To destroy the coactivator binding interaction, preferred mutations are to charged residues (e.g., Arg, Lys, or Glu) on the basis that bulky, surface charged residues might disrupt coactivator binding, yet preserve global receptor
20 structure and solubility. Mutants can be tested for coactivator binding as well as the relative change in strength of the binding interaction. Ligand-dependent coactivator interaction assays also can be tested for this purpose, such as those described herein.

Compounds that bind to the coactivator binding site of nuclear receptors can be identified by computational modeling and/or screening. For example, coactivator agonists or antagonists can be
25 identified by providing atomic coordinates comprising a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system, modeling them, and identifying compounds that fit spacially into the coactivator binding site. By a "portion thereof" is intended the atomic coordinates corresponding to a sufficient number of residues or their atoms of the coactivator binding site that interact with a compound capable of binding to the site. This includes receptor
30 residues having an atom within 4.5Å of a bound compound or fragment thereof. For instance, human TR residues V284, Phe293, Ile302, Leu305 and Leu454 contain side chain atoms that are within 4.5Å, and interact with, hydrophobic residues of a (SEQ ID NO: 1) LxxLL motif of an NR-box 2 coactivator peptide. As another example, an atomic structural model utilized for computational modeling and/or screening of compounds that bind to the coactivator binding site
35 may include a portion of atomic coordinates of amino acid residues corresponding to the site composed of residues of human thyroid receptor selected from Val284, Lys288, Ile302, Lys306, Leu454 and Glu457, or their structural and functional equivalents found in other receptors. Thus,

5 for example, the atomic coordinates provided to the modeling system can contain atoms of the nuclear receptor LBD, part of the LBD such as atoms corresponding to the coactivator binding site or a subset of atoms useful in the modeling and design of compounds that bind to a coactivator binding site.

10 The atomic coordinates of a compound that fits into the coactivator binding site also can be used for modeling to identify compounds or fragments that bind the site. By "modeling" is intended quantitative and qualitative analysis of molecular structure/function based on atomic structural information and receptor-coactivator agonists/antagonists interaction models. This includes conventional numeric-based molecular dynamic and energy minimization models, interactive computer graphic models, modified molecular mechanics models, distance geometry and
15 other structure-based constraint models. Modeling is preferably performed using a computer and may be further optimized using known methods. By "fits spacially" is intended that the three-dimensional structure of a compound is accommodated geometrically by a cavity or pocket of a nuclear receptor coactivator binding site.

20 Compounds of particular interest fit spacially and preferentially into the coactivator binding site. By "fits spacially and preferentially" is intended that a compound possesses a three-dimensional structure and conformation for selectively interacting with a nuclear receptor coactivator binding site. Compounds that fit spacially and preferentially into the coactivator binding site interact with amino acid residues forming the hydrophobic cleft of this site. In particular, the hydrophobic cleft of the coactivator binding site comprises a small cluster of
25 hydrophobic residues. The site also contains polar or charged residues at its periphery. The present invention also includes a method for identifying a compound capable of selectively modulating coactivator binding to different nuclear receptors. The method comprises the steps of modeling test compounds that fit spacially and preferentially into the coactivator binding site of a nuclear receptor of interest using an atomic structural model of a nuclear receptor, screening the test compounds in a
30 biological assay for nuclear receptor activity characterized by preferential binding of a test compound to the coactivator binding site of a nuclear receptor, and identifying a test compound that selectively modulates the activity of a nuclear receptor. Such receptor-specific compounds are selected that exploit differences between the coactivator binding sites of one type of receptor versus a second type of receptor, such as the differences depicted in Figure 19.

35 The invention also is applicable to generating new compounds that distinguish nuclear receptor isoforms. This can facilitate generation of either tissue-specific or function-specific compounds. For instance, GR subfamily members have usually one receptor encoded by a single

5 gene, although there are exceptions. For example, there are two PR isoforms, A and B, translated from the same mRNA by alternate initiation from different AUG codons. There are two GR forms, one of which does not bind ligand. This method is especially applicable to the TR subfamily which usually has several receptors that are encoded by at least two (TR: α , β) or three (RAR, RXR, and PPAR: α , β , γ) genes or have alternate RNA splicing.

10 The receptor-specific compounds of the invention preferably interact with conformationally constrained residues of the coactivator binding site that are conserved among one type of receptor compared to a second type of receptor. "Conformationally constrained" is intended to refer to the three-dimensional structure of a chemical or moiety thereof having certain rotations about its bonds fixed by various local geometric and physical-chemical constraints. Conformationally constrained
15 structural features of a coactivator binding site include residues that have their natural flexible conformations fixed by various geometric and physical-chemical constraints, such as local backbone, local side chain, and topological constraints. These types of constraints are exploited to restrict positioning of atoms involved in receptor-coactivator recognition and binding.

For instance, comparison of sequences of the GR and TR coactivator interaction surface
20 shows a highly negatively charged sequence at the C-terminal end of TR helix 12 (E460 and D461) that is neutral in the equivalent positions in GR helix 12 (GR residues T788 and N759, corresponding to TR residue positions 460 and 461, as depicted in **Figure 19**). As described in the Examples, the cocrystal of the hTR β LBD complexed with the GRIP1 NR-box 2 peptide shows that TR residues E460 and D461 interact with positively charged residues of the NR-box 2 peptide.
25 Also, when comparing the RAR LBD structure to that of the TR LBD, conformation of helix 12 differs slightly, whereas helices 3, 4, 5 and 6 are substantially the same. Thus, differences in helix 12, particularly charge differences at the C-terminal end of the helix, may modulate preferential interaction of TR for NR-box 2 containing coactivators. As further demonstrated in the Examples, TR and GR differ in their specificity for different NR-boxes containing the conserved (SEQ ID NO:
30 1) LxxLL motif found in members of the p160 family of coactivator proteins. As also demonstrated in the Examples, GR but not TR is able to interact with peptides containing the hydrophobic interaction motifs of p53 (SEQ ID NO: 3; FxxLW) and VP16 (SEQ ID NO: 4; FxxAL). Thus, TR exhibits preferential interaction with NR-box peptides comprising the (SEQ ID NO: 1) LxxLL motif, but GR does not discriminate and can bind peptides containing a generic amphipathic helix
35 motif. Accordingly, these real differences among the various nuclear receptors can be exploited in the identification and design of compounds that modulate coactivator binding to one nuclear receptor compared to another.

5 For modeling, docking algorithms and computer programs that employ them can be used to identify compounds that fit into the coactivator binding site. For example, docking programs can be used to predict how a small molecule of interest can interact with the nuclear receptor coactivator binding site. Fragment-based docking also can be used in building molecules *de novo* inside the coactivator binding site, by placing chemical fragments that complement the site to optimize
10 intermolecular interactions. The techniques can be used to optimize the geometry of the binding interactions. This design approach has been made possible by identification of the coactivator binding site structure thus, the principles of molecular recognition can now be used to design a compound which is complementary to the structure of this site. Compounds fitting the coactivator binding site serve as a starting point for an iterative design, synthesis and test cycle in which new
15 compounds are selected and optimized for desired properties including affinity, efficacy, and selectivity. For example, the compounds can be subjected to addition modification, such as replacement and/or addition of R-group substituents of a core structure identified for a particular class of binding compounds, modeling and/or activity screening if desired, and then subjected to additional rounds of testing.

20 Computationally small molecule databases can be screened for chemical entities or compounds that can bind in whole, or in part, to a nuclear receptor coactivator binding site of interest. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity (DesJalais et al., *J. Med. Chem.* (1988) 31:722-729) or by estimated interaction energy (Meng et al., *J. Comp. Chem.* (1992) 13:505-524). The molecule
25 databases include any virtual or physical database, such as electronic and physical compound library databases, and are preferably used in developing compounds that modulate coactivator binding.

Compounds can be designed intelligently by exploiting available structural and functional information by gaining an understanding of the quantitative structure-activity relationship (QSAR),
30 using that understanding to design new compound libraries, particularly focused libraries having chemical diversity of one or more particular groups of a core structure, and incorporating any structural data into that iterative design process. For example, one skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with the coactivator binding site of a nuclear receptor of interest. This process may begin by visual
35 inspection of, for example, the coactivator binding site on the computer screen. Selected fragments or chemical entities may then be positioned into all or part of the site. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and

5 molecular dynamics with standard molecular mechanics force-fields, such as CHARMM and AMBER.

For example, compounds and/or fragments can be designed to fill up the hydrophobic cleft, the pocket deep within the cleft, the upper end of the site, and/or the lower end of the site. Residues comprising a coactivator binding site, when defined by the user as those residues having an atom
10 within 4.5Å of an atom of a bound chemical entity, can be modeled to look for energetic contributions and interaction with the bound chemical entity. For example, a compound or fragment can be designed to contain hydrophobic groups that interact with hydrophobic residues of the coactivator binding site. As described in the examples, human TR residues V284, Phe293, Ile302, Leu305 and Leu454 contain side chain atoms that are within 4.5Å, and interact with,
15 hydrophobic residues of a (SEQ ID NO: 1) LxxLL motif of an NR-box 2 coactivator peptide. Thus, for example, peptides and/or peptide mimetics having a hxxhh motif, where "h" is a hydrophobic residue and x is any residue, can be constructed. Small organic molecules that mimic one or more of these particular interactions also can be designed, for example, by including one or more R-groups that are hydrophobic and fit into the site.

20 Specialized computer programs may also assist in the process of selecting chemical entity fragments or whole compounds. These include: GRID (Goodford, *J. Med. Chem.* (1985) 28:849-857; available from Oxford University, Oxford, UK); MCSS (Miranker et al., *Proteins: Structure, Function and Genetics*, (1991) 11:29-34; available from Molecular Simulations, Burlington, MA); AUTODOCK (Goodsell et al., *Proteins: Structure, Function and Genetics* (1990) 8:195-202;
25 available from Scripps Research Institute, La Jolla, CA); and DOCK (Kuntz et al, *J. Mol. Biol.* (1982) 161:269-288; available from University of California, San Francisco, CA).

Additional commercially available computer databases for small molecular compounds include Cambridge Structural Database and Fine Chemical Database (Rusinko, *Chem. Des. Auto. News* (1993) 8:44-47).

30 Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound. Assembly may be proceeded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of a nuclear receptor. This can be followed by manual model building using software such as Quanta or Sybyl.

5 Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include: CAVEAT (Bartlett et al., "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", In: *Molecular Recognition in Chemical and Biological Problems*", Special Pub., *Royal Chem. Soc.* (1989) 78:182-196; CAVEAT is available from the University of California, Berkeley, CA); 3D Database systems such as MACCS-3D (MDL
10 Information Systems, San Leandro, CA; reviewed in Martin, *J. Med. Chem.* (1992) 35:2145-2154); and HOOK (available from Molecular Simulations, Burlington, MA).

In addition to building a compound in a step-wise fashion, one fragment or chemical entity at a time as described above, compounds that bind to a coactivator binding site of interest also may be designed as a whole or *de novo* using either an empty coactivator binding site or optionally
15 including some portion(s) of a molecule known to binds to the site, such as an NR-box type peptide. These methods include: LUDI (Bohm, *J. Comp. Aid. Molec. Design* (1992) 6:61-78; LUDI is available from Biosym Technologies, San Diego, CA); LEGEND (Nishibata et al., *Tetrahedron* (1991) 47:8985; LEGEND is available from Molecular Simulations, Burlington, MA); and LeapFrog (available from Tripos Associates, St. Louis, MO).

20 Other molecular modeling techniques may also be employed in accordance with this invention. See, for example, Cohen et al., *J. Med. Chem.* (1990) 33:883-894); Navia et al., *Curr. Opin. Struct. Biol.* (1992) 2:202-210). For example, where the structures of test compounds are known, a model of the test compound may be superimposed over the model of the structure of the invention. Numerous methods and techniques are known in the art for performing this step, any of
25 which may be used. See, for example, Farmer, "Drug Design," Ariens, E.J., ed., 10:119-143 (Academic Press, New York, 1980); U.S. Patent No. 5,331,573; U.S. Patent No. 5,500,807; Verlinde, *Structure*, (1994) 2:577-587); and Kuntz et al., *Science*, (1992) 257:1078-1082). The model building techniques and computer evaluation systems described herein are not a limitation on the present invention.

30 Using these computer modeling systems a large number of compounds may be quickly and easily examined and expensive and lengthy biochemical testing avoided. Moreover, the need for actual synthesis of many compounds can be substantially reduced and/or effectively eliminated.

Compounds identified through modeling can be screened in an assay characterized by binding of the compound to a coactivator binding site of interest for coactivator binding activity,
35 such as a biologically based assay. Screening can be *in vitro* and/or *in vivo*. Preferred assays include cell-free competition assays and cell culture based assays. The biological screening

5 preferably centers on activity-based response models, binding assays (which measure how well a compound binds to the receptor), and bacterial, yeast and animal cell lines (which measure the biological effect of a compound in a cell). The assays can be automated for high capacity - high throughput screening (HTS) in which large numbers of compounds can be tested to identify compounds with the desired activity.

10 As an example, *in vitro* binding assays can be performed in which compounds are tested for their ability to block the binding of a coactivator protein, fragment, fusion or peptide thereof, to a coactivator binding site of interest. For cell and tissue culture assays, they may be performed to assess a compound's ability to block function of cellular coactivators, such as members of the p160
15 TIF 2 and NcoA-2, and those that exhibit receptor and/or isoform-specific binding affinity. In a preferred embodiment, compounds of the invention bind to a nuclear receptor coactivator binding site with greater affinity than the cellular coactivator proteins. Tissue profiling and appropriate animal models also can be used to select compounds. Different cell types and tissues also can be used for these biological screening assays. Suitable assays for such screening are described herein
20 and in Shibata et al. (*Recent Prog. Horm. Res.* 52:141-164 (1997)); Tagami et al. (*Mol. Cell Biol.* (1997) 17(5):2642-2648); Zhu et al. (*J. Biol. Chem.* (1997) 272(14):9048-9054); Lin et al. (*Mol. Cell Biol.* (1997) 17(10):6131-6138); Kakizawa et al. (*J. Biol. Chem.* (1997) 272(38):23799-23804); and Chang et al. (*Proc. Natl. Acad. Sci. USA* (1997) 94(17):9040-9045), which references are incorporated herein in their entirety by reference. For example, coactivators or binding fragments
25 thereof can be expressed and/or assayed for binding as for GRIP1 (Hong et al., *MCB supra*; and Hong et al., *PNAS supra*) and/or SRC-1 (Spencer et al., *Nature* (1997) 389:194-198; Onate et al., *Science* (1995) 270:1354-1357), incorporated by reference.

The compounds selected can have agonist and/or antagonistic properties. The compounds also include those that exhibit new properties with varying mixtures of agonist and antagonist
30 activities, depending on the effects of altering coactivator binding in the context of different activities of nuclear receptors, either hormone-dependent or hormone-independent, which are mediated by proteins other than coactivators, and which interact with the receptors at locations other than the coactivator binding site. The compounds also include those, which through their binding to receptor locations that are conformationally sensitive to hormone binding, have allosteric
35 effects on the receptor by stabilizing or destabilizing the hormone-bound conformation of the receptor, or by directly inducing the same, similar, or different conformational changes induced in the receptor by the binding of hormone.

5 Of particular interest is use of such compounds in a method of modulating nuclear receptor activity in a mammal by administering to a mammal in need thereof a sufficient amount of a compound that fits spatially and preferentially into a coactivator binding site of a nuclear receptor of interest. By "modulating" is intended increasing or decreasing activity of a nuclear receptor. For example, pre-clinical candidate compounds can be tested in appropriate animal models in order to
10 measure efficacy, absorption, pharmacokinetics and toxicity following standard techniques known in the art. Compounds exhibiting desired properties are then tested in clinical trials for use in treatment of various nuclear receptor-based disorders. These include ER-based disorders, such as postmenopausal symptoms and cancer resulting from loss of estrogen production, and osteoporosis and cardiovascular disease stemming from traditional estrogen replacement therapy. Others include
15 TR-based disorders including cardiovascular disease, metabolic disorders, hyperthyroidism, glaucoma and skin disorders. GR-based disorders include Type II diabetes and inflammatory conditions such as rheumatic diseases.

 The invention also provides for cocrystals made from nuclear receptor ligand binding domains with a molecule bound to the coactivator binding site. As exemplified in the Examples,
20 TR LBDs are co-crystallized with a peptide molecule comprising a coactivator NR-box 2 peptide sequence bound to the coactivator binding site, and the hormone/ligand T₃.

 Crystals are made from purified nuclear receptor LBDs that are usually expressed by a cell culture, such as *E. coli*. Preferably, different crystals (cocrystals) for the same nuclear receptor are separately made using different coactivators-type molecules, such as protein fragments, fusions or
25 small peptides. The coactivator-type molecules preferably contain NR-box sequences necessary for binding to the coactivator binding site, or derivatives of NR-box sequences. Other molecules can be used in co-crystallization, such as small organics that bind to the coactivator or hormone binding site(s). Heavy atom substitutions can be included in the LBD and/or a co-crystallizing molecule.

 After the three dimensional structure of the cocrystal is determined, the structural
30 information can be used in computational methods to design synthetic compounds for the nuclear receptor, and further structure-activity relationships can be determined through routine testing using the assays described herein and known in the art.

 Since nuclear receptor LBDs may crystallize in more than one crystal form, the structure coordinates of such receptors or portions thereof, as provided in **Appendix 1**, are particularly useful
35 for solving the structure of those other crystal forms of nuclear receptors. They may also be used to

- 5 solve the structure of mutants or co-complexes of nuclear receptors having sufficient structural similarity.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, may be determined using the structure coordinates of this invention as provided in Appendix 1. This method will provide an accurate structural form for the
10 unknown crystal more quickly and efficiently than attempting to determine such information *ab initio*.

Atomic coordinate information gleaned from the crystals of the invention can be stored. In a preferred embodiment, the information is provided in the form of a machine-readable data storage medium. This medium contains information for constructing and/or manipulating an atomic model
15 of a coactivator binding site or portion thereof. For example, the machine readable data for the coactivator binding site comprises structure coordinates of amino acids corresponding to human TR amino acids selected from C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459), or a homologue of the molecule or molecular
20 complex comprising the site. The homologues comprise a coactivator binding site that has a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å. A preferred molecule or complex represents a compound bound to the coactivator binding site.

The machine-readable data storage medium can be used for interactive drug design and molecular replacement studies. For example, a data storage material is encoded with a first set of
25 machine-readable data that can be combined with a second set of machine-readable data. For molecular replacement, the first set of data can comprise a Fourier transform of at least a portion of the structural coordinates of the nuclear receptor or portion thereof of interest, and the second data set comprises an X-ray diffraction pattern of the molecule or molecular complex of interest. Using a machine programmed with instructions for using the first and second data sets a portion or all of
30 the structure coordinates corresponding to the second data can be determined.

Protein for crystals and assays described herein can be produced using expression and purification techniques described herein and known in the art. For example, high level expression of nuclear receptor LBDs can be obtained in suitable expression hosts such as *E. coli*. Expression of LBDs in *E. coli*, for example, includes the TR LBD and other nuclear receptors, including
35 members of the steroid/thyroid receptor superfamily, such as the receptors ER, AR, MR, PR, RAR, RXR and VDR. Yeast and other eukaryotic expression systems can be used with nuclear receptors

5 that bind heat shock proteins as these nuclear receptors are generally more difficult to express in bacteria, with the exception of ER, which can be expressed in bacteria. Representative nuclear receptors or their ligand binding domains have been cloned and sequenced: human RAR- α , human RAR- γ , human RXR- α , human RXR- α , human PPAR- α , human PPAR- β , human PPAR- γ , human VDR, human ER (as described in Seielstad *et al.*, *Molecular Endocrinol.*, (1995) 9:647-658,
10 incorporated herein by reference), human GR, human PR, human MR, and human AR. The LBD for each of these receptors has been identified.

Coactivator proteins can be expressed using techniques known in the art, particularly members of the p160 family of coactivator proteins that have been cloned and/or expressed previously, such as SRC-1, AIB1, RAC3, p/CIP, and GRIP1 and its homologues TIF 2 and NcoA-2.
15 A preferred method for expression of coactivator protein is to express a fragment that retains transcriptional activation activity using the "yeast 2-hybrid" method as described by Hong *et al.* (*PNAS supra*; and *MCB supra*), for GRIP1 expression, which reference is herein incorporated by reference.

The proteins can be expressed alone, as fragments of the mature or full-length sequence, or
20 as fusions to heterologous sequences. For example, TR can be expressed without any portion of the DBD or amino-terminal domain. Portions of the DBD or amino-terminus can be included if further structural information with amino acids adjacent the LBD is desired. Generally, for the TR the LBD used for crystals will be less than 300 amino acids in length. Preferably, the TR LBD will be at least 150 amino acids in length, more preferably at least 200 amino acids in length, and most
25 preferably at least 250 amino acids in length. For example the LBD used for crystallization can comprise amino acids spanning from Met 122 to Val 410 of the rat TR- α or Glu 202 to Asp 461 of the human TR- β .

Typically the LBDs are purified to homogeneity for crystallization. Purity of LBDs can be measured with sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE), mass
30 spectrometry (MS) and hydrophobic high performance liquid chromatography (HPLC). The purified LBD for crystallization should be at least 97.5 % pure, preferably at least 99.0% pure, more preferably at least 99.5% pure.

Initially, purification of the unliganded receptor can be obtained by conventional techniques, such as hydrophobic interaction chromatography (HPLC), ion exchange chromatography (HPLC),
35 and heparin affinity chromatography.

5 To achieve higher purification for improved crystals of nuclear receptors, especially the TR subfamily and TR, the receptors can be ligand-shift-purified using a column that separates the receptor according to charge, such as an ion exchange or hydrophobic interaction column, and then bind the eluted receptor with a ligand, especially an agonist. The ligand induces a change in the receptor's surface charge such that when re-chromatographed on the same column, ligand-bound
10 receptor is separated from unliganded receptor. Usually saturating concentrations of ligand are used in the column and the protein can be preincubated with the ligand prior to passing it over the column. The structural studies detailed herein indicate the general applicability of this technique for obtaining super-pure nuclear receptor LBDs for crystallization.

Purification can also be accomplished by use of a purification handle or "tag," such as with
15 at least one histidine amino acid engineered to reside on the end of the protein, such as on the N-terminus, and then using a nickel or cobalt chelation column for purification. (Janknecht et al., *Proc. Natl. Acad. Sci. USA*, (1991) 88:8972-8976) incorporated by reference.

Typically purified LBD, such as TR LBD, is equilibrated at a saturating concentration of ligand at a temperature that preserves the integrity of the protein. Ligand equilibration can be
20 established between 2 and 37°C, although the receptor tends to be more stable in the 2-20°C range. Preferably crystals are made with the hanging drop methods detailed herein. Regulated temperature control is desirable to improve crystal stability and quality. Temperatures between 4 and 25°C are generally used and it is often preferable to test crystallization over a range of temperatures. The crystals are then subjected to vapor diffusion and bombarded with x-rays to obtain x-ray diffraction
25 pattern following standard procedures.

For co-crystallization with a peptide that binds to the coactivator binding site, various concentrations of peptides containing a sequence that binds to a coactivator binding site of a nuclear receptor of interest can be used in microcrystallization trials, and the appropriate peptides selected for further crystallization. Any number of techniques, including those assays described herein can
30 assay peptides for binding to the coactivator binding site of a nuclear receptor of interest. In a preferred embodiment, a NR-box 2 sequence-containing peptide is used for crystallization with TR LBD. A preferred peptide contains a NR-box (SEQ ID NO: 1) LxxLL motif, and suitable flanking sequences necessary for binding and forming complex with coactivator binding site of the nuclear receptor of interest, such as a TR LBD. The binding peptides are then tested in crystallization trials
35 at various concentrations and ratios of concentrations with a nuclear receptor of interest, for example, as described herein and in the Examples. For crystallization trials with TR LBD, the hanging drop vapor diffusion method is preferred. Conditions of pH, solvent and solute

5 components and concentrations and temperature can be adjusted, for instance, as described in the Examples. In the hanging drop method, to obtain suitable crystals for x-ray diffraction analysis, seeding of prepared drops with microcrystals of the complex can be used. Collection of structural information can be determined by molecular replacement using the structure of TR LBD determined herein or previously by Wagner et al., supra. The structure is refined following
10 standard techniques known in the art.

There are many uses and advantages provided by the present invention. For example, the methods and compositions described herein are useful for identifying peptides, peptidomimetics or small natural or synthetic organic molecules that modulate nuclear receptor activity. The compounds are useful in treating nuclear receptor-based disorders. Methods and compositions of
15 the invention also find use in characterizing structure/function relationships of natural and synthetic coactivator compounds.

The following examples illustrate various aspects of this invention. These examples do not limit the scope of this invention.

5

EXAMPLES**Example 1: Expression and purification of wild-type and mutant nuclear receptors and coactivators****A. Human TR β LBD**

Human TR β LBD (His6-E202-D461) was expressed and purified as described (Shiau et al., *Gene* (1996) 179(2):205-10). Briefly, the protein was expressed from pET (e.g., pET3 and pET28) in BL21DE3 at 14°C, induced at OD(600nm) 0.7 with 1mM IPTG and incubation was extended for 24 hours. Cells were harvested and lysed in 50mM sodium-phosphate buffer (pH 8.0), 0.3M NaCl, 10% glycerol, 25mM β -mercaptoethanol and 0.1mM PMSF as described above. The lysate was cleared by ultracentrifugation (Ti45, 36000 rpm, 1h, 4°C), loaded on a Talon column equilibrated in the sodium phosphate buffer described above, washed with 12mM imidazole and eluted with an imidazole gradient (12 - 300 mM). TR β LBD containing fractions were loaded in 0.6M ammonium sulfate on a TSK-phenyl hydrophobic interaction column and eluted with a reverse ammonium sulfate gradient [0.6 - 0 M] in 50% glycerol and 10% acetonitrile. Fractions containing TR β LBD were tested for hormone binding, pooled and incubated with a 3-fold molar excess of T₃ (Sigma). The hydrophobic interaction run was repeated with liganded receptor under the same conditions. Liganded receptor, which elutes earlier than unliganded receptor, was collected and buffer changed to 20mM Hepes pH7.0, 3mM DTT and 0.1 μ M T₃ using NAP columns (Pharmacia). For crystallization, the protein was concentrated by ultrafiltration (Millipore UFV2BGC10 concentrators) to a final concentration of 9mg/ml. The yield was about 9.5mg protein per liter bacterial culture.

B. Human TR mutants

Thirty-seven thyroid receptor mutants were created by synthesizing double-stranded oligonucleotides which encode the mutant sequence and which have ends allowing them to be ligated as a cassette using pairs of the NsiI, PstI, SstI, AlwNI, ApoI, PflMI, BstXI, BseRI, BsmFI, PvuII, NspI, SmaI, PmlI, BglII and BsmI restriction sites of the hTR β 1 cDNA sequence, or the 3' plasmid polylinker SalI, or BamHI restriction sites. The hTR β 1 sequences thus mutated were subcloned into the pCMX vector encoding the full-length 461 amino acid hTR β 1 sequence. Some of the mutations of the hTR β 1 in the CMX vector and all three mutations of the hER α in the pSG5-ER-HEGO vector (Tora et al., *EMBO* (1989) 8:1981) were created using Quick Change Site-

- 5 Directed Mutagenesis Kits (Stratagene). The mutated sequences were verified by DNA sequencing using Sequenase Kits (Stratagene).

C. Human ER α LBD

- The human ER α -LBD 297-554 was overexpressed as described previously (Seielstad, et al., *supra*) in BL21(DE3)pLysS cells transformed with a modified pET-23d-ERG vector that contained
10 the sequence Met-Asp-Pro fused to residues 297 to 554 of the hER α (provided by Paul Sigler of Yale University). Clarified bacterial lysates were adjusted to 3 M in urea and 0.7 M in NaCl and then applied to a 10-ml column of estradiol-Sepharose (Greene, et al., *Proc. Natl. Acad. Sci. USA* (1980) 77:5115-5119; Landel, et al., *Mol. Endocrinol.* (1994) 8:1407-1419; Landel, et al., *J. Steroid Biochem. Molec. Biol.* (1997) 63:59-73).
- 15 To carboxymethylate the solvent-accessible cysteines, the bound hER α -LBD was treated with 5 mM iodoacetic acid in 10 mM Tris, pH 8.1, 250 mM NaSCN (Hegy, et al., *Steroids* (1996) 61:367-373). Protein was eluted with 3 x 10⁻⁵ M ligand (either DES or OHT) in 30-100 ml of 50 mM Tris, 1 mM EDTA, 1 mM DTT and 250 mM NaSCN, pH 8.5. The yield of hER α -LBD was typically close to 100% (Seielstad, et al., *Biochemistry* (1995) 34:12605-12615). The affinity-
20 purified material was concentrated and exchanged into 20 mM Tris, 1 mM EDTA, 4 mM DTT, pH 8.1 by ultrafiltration. The protein was bound to a Resource Q column (Pharmacia) and then eluted with a linear gradient of 25-350 mM NaCl in 20 mM Tris, pH 8.1, 1 mM DTT. The hER α -LBD-ligand complexes eluted at 150-200 mM NaCl. Pooled fractions were concentrated by ultrafiltration and analyzed by SDS-PAGE, native PAGE, and electrospray ionization mass
25 spectrometry.

D. Human ER mutants

- To test the importance of the NR box peptide/LBD interface observed in the crystal, a series of site-directed mutations were introduced into the ER α LBD. These mutations were designed either to simultaneously perturb the structural integrity and the nonpolar character of the floor of the
30 binding groove (Ile 358->Arg, Val 376->Arg and Leu 539->Arg) or to prevent the formation of the capping interactions (Lys 362->Ala and Glu 542->Lys). Fusions of glutathione-S-transferase (GST) to the wild-type and mutant LBDs were analyzed for their ability to bind ³⁵S-labeled GRIP1 in the absence of ligand or in the presence of DES or OHT.

5 ³⁵S-labeled GRIP1 was incubated with either immobilized GST, immobilized wild type
GST-hER α LBD, or immobilized mutant GST-LBDs in the absence of ligand or in the presence of
DES or OHT. The bound GRIP1 was quantitated after SDS-PAGE. I358R, mutant LBD
containing a Ile->Arg substitution at residue 358; K362A, mutant LBD containing a Lys->Ala
substitution at residue 362; V376R, mutant LBD containing a Val->Arg substitution at residue 376;
10 L539R, mutant LBD containing a Leu->Arg substitution at residue 539; E542K, mutant LBD
containing a Glu->Lys substitution at residue 542.

In the absence of ligand or in the presence of OHT, fusions to the wild-type protein and all
of the mutant LBDs showed no detectable binding to GRIP1. The Ile 358->Arg, Val 376->Arg and
Leu 539->Arg mutants were all unable to interact with coactivator in the presence of agonist,
15 confirming the importance of the packing interactions observed in the crystal. Disruption of either
the N- or C-terminal capping interaction also compromised GRIP1 binding in the presence of
agonist. Only the wild-type GST-LBD was able to recognize the coactivator in the presence of
DES.

E. Human ER LBD-GST Fusion Protein

20 A fusion between glutathione-S-transferase (GST) and amino acids 282-595 of hER α was
constructed by subcloning the EcoRI fragment from pSG5 ER α -LBD (Lopez et al., submitted
manuscript) into pGEX-3X (Pharmacia). The Ile 358-> Arg, Lys 362->Ala, and Leu 539->Arg
mutations were introduced into the GST-LBD construct using the QuikChange Kit (Stratagene)
according to the manufacturer's instructions. The Val 376->Arg and Glu 542->Lys mutations were
25 created in the GST-LBD construct by subcloning the BsmI/HindIII fragments of derivatives of
pSG5-ER-HEGO (Tora, et al., *supra*) into which these mutations had already been introduced. All
constructs were verified by automated sequencing (University of Chicago Cancer Research Center
DNA Sequencing Facility).

F. Radiolabeled full-length receptors and coactivator proteins

30 Wild-type (WT) or mutant pCMV-hTR β 1 vector and the pSG5-GRIP1 and pCMX-SRC-1a
vectors were used to produce radiolabeled full-length receptors and coactivator proteins using the
TNT coupled Reticulocyte Lysate System (Promega) and [³⁵S]-Met (DuPont). GST-GRIP1 (amino
acids 721-1221), GST-GRIP1 (amino acids 563-1121), GST-SRC-1a (amino acids 381-882), GST-
hTR β 1 (full-length, WT or mutants, WT provided by. C. Costa), and the GST-hRXR α (full-length

- 5 provided by. C. Costa), fusion proteins were produced in *E. coli* strain HB101 as per the manufacturer's protocol (Pharmacia Biotech).

G. Coactivator GRIP1 563-767 His6 GST fusion protein

- GRIP1 563-767 was cloned as a Bam HI-Xho I fragment derived from pGEX-2TK GRIP1 563-1121 into the corresponding sites of pGEX-4T1. A His6-tag was added by inserting a Xho I-Nae I fragment of pET23a into Xho I-Bsa AI sites of this pGEX-4T1 construct yielding pGEX GRIP1 563-767His6. Mutants of GRIP1 563-767 were generated by PCR or single stranded mutagenesis using oligonucleotides carrying the mutations and a pSG5 GRIP1 vector as template. The mutations were confirmed by sequence analysis and integrated into pGEX GRIP1 563-767His6 as NgoMI - Xho I fragments. The GRIP1 563-767 His6 GST fusion protein was expressed in HB101 at 37°C. Protein expression was induced with 1mM IPTG at an optical density (600 nm) of 0.7 and extended for 4 hours after induction. Cells were harvested by centrifugation, resuspended in sonication buffer (20mM TrisHCl pH 8.0, 0.1M NaCl, 10%glycerol, 0.1mM PMSF and protease inhibitors (Complete, EDTA free, Boehringer Mannheim)). The resuspended cells were freeze-thawed once, incubated on ice with 0.1mg/ml lysozyme for 20 minutes and lysed per sonication. The lysate was cleared by ultracentrifugation (Ti 45, 36000rpm, 1h 4°C), the supernatant filtered (Costar 0.2µm top filter) and loaded on a Talon column (Clontech). The column was washed with 10 column volumes of sonication buffer supplemented with 12mM imidazole and eluted with an imidazole gradient [12 - 100mM]. At this step the fusion proteins are about 95% pure. Imidazole was removed by gelfiltration on NAP columns (Pharmacia), and protein concentrations determined using the Biorad protein assay. Equal concentrations of the different derivatives of the fusion fragment were incubated with glutathione agarose (1h, 4°C) which was equilibrated in binding buffer (sonication buffer supplemented with 1mM DTT, 1mM EDTA and 0.01% NP-40). Beads were washed with at least 20 volumes of this buffer, diluted in binding buffer with 20% glycerol to 40%, frozen in aliquots and stored at -70°C.

H. Coactivator GRIP1 563-767 His6

- GRIP1 563-767 was cloned as a Bam HI - Xho I fragment derived from pGEX GRIP1 563-767His6 into corresponding cloning sites of pET23a yielding pETGRIP1 563-767His6. The fragment was expressed in BL21DE3. Expression, cell lysis and Talon purification was identical as described for GST GRIP1 563-767His6. The protein eluted from a Talon column in two fractions, one at 12mM and one between 40 and 70mM imidazole. In the earlier eluting fraction the fragment was associated with a 70 kDa protein which was removed by a MonoQ run in 50mM TrisHCl

- 5 pH7.5, 10% glycerol, 1mM EDTA, 1mM DTT, 0.1mM PMSF and protease inhibitors. GRIP1 563-767His6 eluted in the flow through and was concentrated by ultrafiltration. At this step the protein was more than 95% pure.

Example 2: Peptide synthesis

- 10 Coactivator peptides were obtained using standard techniques. All peptides were HPLC purified and analyzed by mass spectroscopy. Peptide concentrations were either determined spectroscopically using the tyrosine signal ($A_{276} = 1450 \text{ M}^{-1}\text{cm}^{-1}$) or by amino acid analysis following standard techniques.

Example 3: Binding assays with nuclear receptors and coactivators

A. GST-GRIP Pull-down Assays and Peptide Competition Assays

- 15 Binding experiments were performed by mixing glutathione beads containing 10 μg of GST fusion proteins (Coomassie Plus Protein Assay Reagent, Pierce) with 1-2 μl of the [^{35}S]-labeled wild-type or mutant hTR β 1 (25 fmoles, 4000 cpm of receptor), or coactivators in 150 μl of binding buffer (20 mM HEPES, 150 mM KCl, 25 mM MgCl_2 , 10% glycerol, 1 mM dithiothreitol, 0.2 mM phenylmethylsulfonyl fluoride, and protease inhibitors) containing 2 mg/ml BSA for 1.5 hrs in the
20 presence or absence of 1 μM T_3 . Beads were washed 3 times with 1 ml of binding buffer and the bound proteins were separated using 10% SDS-PAGE and visualized by autoradiography. Binding was quantitated by phosphorimaging using ImageQuant (Molecular Dynamics).

- For *in vitro* binding studies GR, TR and their derivatives were translated in the presence of [^{35}S]methionine using the TNT Coupled Reticulocyte System (Promega). Separate translations were
25 performed in the presence and absence of 10 μM dexamethasone or 1 μM RU486 for GR and 10 μM triiodothyronine for TR. Expression was quantified by phosphorimager analysis (BAS2000, Fuji). For all binding assays 50 μl of a 20% bead suspension containing either 1.6 or 4.0 μM bound purified GST GRIP1 fragment (either 568-767 or 563-1121) was incubated with 0.2 μl or 1.4 μl *in vitro* transcribed and translated TR or GR, respectively. Binding was performed in the binding
30 buffer described above supplemented with 20 $\mu\text{g}/\text{ml}$ BSA and appropriate hormone. The chosen GST GRIP1 fragment concentrations were sufficient to bind either 70 or 100% of the TR derivatives. The reaction was incubated at 4°C under rotation for 2 hours. In case of competition experiments, the appropriate concentration of peptides were added to the reaction before addition of

5 receptors. However, no differences in the results were noted by adding the peptides after half of the incubation of the GST GRIP1 fragment with nuclear receptors. This demonstrates that equilibrium is reached under the chosen conditions. Beads were washed five times with 200 μ l binding buffer + BSA at 4°C before elution of the bound proteins in 20 μ l SDS loading buffer. Eluted beads and input labeled protein were subjected to SDS-PAGE. The fraction of bound nuclear receptors was
10 determined by phosphorimager analysis.

B. GST-hTR β 1 Pull-down Assays

Assay and analysis was performed as for Example 3A. *In vitro* binding of [35 S]-labeled full-length GRIP1, [35 S]-labeled full-length SRC-1a, and [35 S]-labeled full-length hRXR α , to GST-hTR β 1 wild-type (WT) and mutants was performed. Mutants V284R, K288A, I302R, L454R, and
15 E457K all bound to hRXR α with an affinity equivalent to wild type hTR. All of these mutants showed decreased ability to bind GRIP1 and SRC-1a, as expected from the results of Example 3A. The same results were obtained when a GST-SRC1 construct including SRC-1a amino acids 381-882 was tested for binding of [35 S]-Met-labeled full-length hTR β 1 WT and mutants (data not shown).

20 C. GST-hER α LBD Pull-down Assays

The wild-type and mutant GST-hER α LBDs were expressed in BL21(DE3) cells. Total ligand binding activity was determined by a controlled pore glass bead assay (Greene, et al., *Mol. Endocrinol.* (1988) 2:714-726) and protein levels were monitored by western blotting with a monoclonal antibody to hER α (H222). Cleared extracts containing the GST- hER α LBDs were
25 incubated in buffer alone (50 mM Tris, pH 7.4, 150 mM NaCl, 2 mM EDTA, 1 mM DTT, 0.5% NP-40 and a protease inhibitor cocktail) or with 1 μ M of either DES or OHT for 1 hour at 4°C. Extract samples containing thirty pmol of GST-LBD were then incubated with 10 μ l glutathione-Sepharose-4B beads (Pharmacia) for 1 hour at 4°C. Beads were washed five times with 20 mM HEPES, pH 7.4, 400 mM NaCl, and 0.05% NP-40. 35 S-labeled GRIP1 was synthesized by *in vitro*
30 transcription and translation using the TNT Coupled Reticulocyte Lysate System (Promega) according to the manufacturer's instructions and pSG5-GRIP1 as the template. Immobilized GST-hER α LBDs were incubated for 2.5 hours with 2.5 μ l aliquots of crude translation reaction mixture diluted in 300 μ l of Tris-buffered saline (TBS). After five washes in TBS containing 0.05% NP-40,

- 5 proteins were eluted by boiling the beads for 10 minutes in sample buffer. Bound ^{35}S -GRIP1 was quantitated by fluorography following SDS-PAGE.

D. Electrophoretic Mobility Shift Assays

- GRIP1, a mouse p160 coactivator, recognizes the ER α LBD in a ligand-dependent manner. The binding of agonists to the ER α LBD promotes recruitment of GRIP1, whereas binding of
10 antagonists prevents this interaction (Norris, et al., *J. Biol. Chem.* (1998) 273:6679-88). While agonist-bound receptor will bind to all three of the NR boxes from GRIP1, ER α strongly prefers NR-box 2 (Ding, et al., *Mol. Endocrinol.* (1998) 12:302-13).

- An electrophoretic mobility shift assay was used to directly assess the ability of the NR-box 2 peptide to bind the purified ER α LBD in the presence of either DES or OHT. Eight microgram
15 samples of purified hER α -LBD bound to either DES or OHT were incubated in the absence of the peptide, i.e., buffer alone, or in the presence of either a 2-fold or 10-fold molar excess of the GRIP1 NR-box 2 peptide. The binding reactions were performed on ice for 45 minutes in 10 μl of buffer containing 20mM Tris, pH 8.1, 1mM DTT, and 200mM NaCl and then subjected to 6% native PAGE. Gels were stained with GELCODE Blue Stain reagent (Pierce).

- 20 In the presence of the NR-box 2 peptide, the migration of the DES-hER α -LBD complex was retarded. In contrast, peptide addition had no effect on the mobility of the OHT-hER α -LBD complex. Hence, this peptide fragment of GRIP1 possesses the ligand-dependent receptor binding activity characteristic of the full-length protein.

Example: 4 Transfection assays with TR and hER α

- 25 HeLa cell transfection and assay conditions are described (Webb et al., *Mol Endocrinol* (1995) 9:443). For TR assays, 5 μg of the reporter p(DR-4) $_2$ -TK-LUC consisting of two copies of the DR-4 element (a direct repeat of the consensus TR response element (TRE) spaced by 4 base pairs) placed upstream of a minimal (-32/+45) thymidine kinase gene promoter linked to luciferase (LUC) coding sequences were used. A reporter containing palindromic TREs gave the same results
30 (data not shown). Also, 2 μg of the hTR β 1 expression vector, pCMX-TR (WT or mutant), and 0.5 μg transfection control vector, pJ3LacZ, which contains the SV40 promoter linked to the β -galactosidase gene. were used. Other cells co-transfected with vector or receptor constructs can be used for same purpose. Alternative cells expressing sufficient levels of an endogenous receptor(s),

- 5 or cells selected that express a single reporter, can be used for transfection assays, including MCF-7 cells expressing ER (Webb et al., *supra*), and GC cells expressing TR (Norman et al., *J. Biol. Chem.* (1989) 264:12063-12073).

For hER α assays, 5 μ g of estrogen responsive reporter plasmid encoding chloramphenicol acetyltransferase (CAT), pERE-collTATA (Sadovsky, *et al.*, *Mol Cell Biol.* (1995) 15:1554), 0.5 μ g expression vector encoding full-length hER α , pSG5-er HEGO (WT or mutants), and 2 μ g of pj3lacZ, were used. For the experiments of Figures 2 and 4, 0.5 μ g of a full-length GRIP1 expression vector, pSG5-GRIP1, was also included in the transfection. Transfected cells were treated with or without 1 μ M T₃ or E₂, as indicated. After culturing for 24 hrs, the LUC or CAT activities were assayed and the β -galactosidase activities were also assayed to correct for differences in transfection efficiencies. The triplicate points were averaged and standard deviations were less than 10%.

Example 5: Hormone binding assays for wild-type and mutant TRs

The T₃ binding affinity constants (K_d) for *in vitro* -translated WT and mutant TRs were measured using [¹²⁵I] 3,5,3' triiodo-L-thyronine ([¹²⁵I]T₃) in gel filtration binding assays as described (Apriletti et al., *Protein Expr. Purif.* (1995) 6:363). Both the K_d and standard error (S.E.) values were calculated using the Prism computer program (GraphPad Software, Inc.). Mutations are indicated by the single-letter amino acid abbreviations, with the native residue name, followed by the primary sequence position number, and then the mutated residue name. The affinity of the WT TR is 81 \pm 12 pM. The relative affinity was determined by dividing the WT K_d by each mutant K_d. The 37 mutants tested with their relative affinities are: E217R (123%), E227R (109%), K242E (92%), E267R (117%), H271R (123%), T277R (7%), T281R (145%), V284R (105%), D285A (89%), K288A (98%), C294K (94%), E295R (118%), C298A (87%), C298R (141%), E299A (171%), I302A (86%), I302R (99%), K306A (6%), K306E (6%), P384R (164%), A387R (107%), E390R (151%), E393R (146%), L400R (95%), H413R (109%), H416R (153%), M423R (156%), R429A (48%), S437R (170%), L440R (174%), V444R (89%), T448R (234%), E449R (36%), P453E (32%), L454R (26%), L456R (46%), E457K (71%).

Example 6: Coactivator binding assays for wild-type and mutant TRs

Wild type (WT) TR and most of the TR mutants liganded to 3,5,3'-triiodo-L-thyronine (T₃) bind equally well to the coactivator, GRIP1. In all cases, GRIP1 binding was hormone-dependent

5 (data not shown). Mutations L454R and E457K in surface residues of helix 12 abolish GRIP1 binding (**Figure 1**). Mutations in two residues of helix 3, V284R and K288A, and two residues of helix 5, I302R and K306A, also impair binding (**Figure 1**). Five mutations with diminished GRIP1 binding (V284R, K288A, I302R, L454R, and E457K) also show decreased binding to another coactivator, SRC-1a (data not shown). Thus, these results show that two different coactivators
10 recognize the same TR surface residues.

Example 7: TR residues involved in ligand-dependent transcription activation in context of a cell

Residues involved in ligand-mediated transcription activation were identified by testing the TR mutants of Example 8 in HeLa cells. T₃ increased reporter gene activity 5-fold in cells
15 expressing either WT TR or mutated TRs showing normal GRIP1 binding (representative mutants are shown in **Figure 1**). By contrast, TR mutants with diminished or absent GRIP1 binding (V284R, K288A, I302R, K306A, L454R, and E457K) show a diminished or absent response to T₃ which correlates with the GRIP1 binding defect. Overexpression of GRIP1 increases activation by the WT TR and rescues activation by TR mutants roughly in proportion to the severity of the defect of
20 GRIP1 binding and activation (**Figure 2**). These results suggest that the same residues are required for coactivator binding, function of the endogenous coactivator(s) in HeLa cells, and responsiveness of TRs to GRIP1.

Example 8: Effect of TR mutations on other receptor functions

The effects of the mutations on other receptor functions also were examined. All of the
25 mutants bound radiolabeled thyroid hormone (K_d values, 6%-234% that for native receptor); occasional lower values were expected because some residues have partially buried side chains. None of the residues that decrease GRIP1 binding affected TR binding to a GST-RXR fusion protein or to DNA using three different DNA half-site arrangements and testing with or without added RXR (data not shown). Some mutations that affect GRIP1 binding occur in a region
30 spanning helices 3-5, which has been suggested as important for TR/RXR heterodimerization (O'Donnell et al., *supra*; Lee et al., *Mol. Endocrinol.* (1992) 6:1867-1873). In contrast, however, the above results indicate that these residues do not contribute to TR/RXR heterodimerization. Further, TRs mutated in the CBS residues retain the ability of WT TR of T₃-dependent inhibition of the activity of the Jun and Fos transcription factors at an AP-1 site (Saatcioglu et al., *supra*), suggesting
35 that the CBS residues do not participate in TR actions mediated through these proteins. These data

- 5 indicate that the mutational effects are specific, the amount of input labeled TR in the different reactions is comparable, and the levels of expression of the mutant TRs are comparable to those of WT receptors.

Example 9: Coactivator binding site in ER

- 10 Three separate mutations (K362A, V376R, and E542K) were created in human estrogen receptor- α (hER α) which align to three of the effective positions in hTR β 1 (K288A, I302R, and E457K). All three mutations diminish GRIP1 binding and abolish transcriptional activation (Figure 3), and mutant V376R, with 10% residual GRIP1 binding, was rescued partially by overexpression of GRIP1 (Figure 4). As a control, the ER mutants demonstrated a normal hormone-dependent ability to activate a vitellogenin-LUC hybrid reporter gene, GL45, which
15 responds to the ER amino-terminal activation function (Berry et al., *EMBO J* (1990) 9:2811-2818) (data not shown). The finding that similar residues are required for GRIP1 binding and transcription activation activity in the TR and ER suggests that the coactivator binding site residues are similar in different nuclear receptors.

Example 10: Coactivator NR-box binding affinity for TR

- 20 To study the interaction between nuclear receptors and GRIP1 *in vitro*, a fragment of GRIP1 (563-767) was purified that contains all three NR-boxes (Figures 6 and 7). The fragment was found to be highly soluble and, in agreement with a secondary structure prediction using PhD, displays a mainly alpha-helical far UV-CD spectrum (data not shown). Three of the four helices predicted for the fragment include the NR-boxes at their C-terminus, suggesting that these boxes are
25 part of amphipathic alpha-helices. These results show that the NR-boxes of GRIP1 are contained in a soluble, alpha-helical 24kD fragment.

- Binding assays show that GRIP1 NR-boxes 1, 2 and 3, interact differentially with hTR β LBD (Figure 7). A GST-fusion of the GRIP1 (563-767) fragment strongly binds TR (kD or EC50) in a ligand depend fashion. Replacement of the hydrophobic residues of NR-box 3 with alanine
30 does not reduce binding of TR significantly, whereas similar replacement of NR-box 2 results in loss of TR binding of about 50%. By titrating the amount of GRIP1 fragment, about a 4-fold stronger binding of TR for NR-box 2 (EC50 = 1.0 μ M) over NR-box 3 (EC50 = 4.0 μ M) was estimated. In the absence of functional NR-boxes 2 and 3, almost no binding to TR was detected suggesting that under these experimental conditions NR-box 1 is not a cognate binding site for TR.

- 5 Full length TR or TR-LBD bound GRIP1 equally. These results show that TR recognizes GRIP1 NR-box 2 and 3, with preference for NR-box 2.

Example 11: Coactivator NR-box binding affinity for GR

- GR also was found to bind GRIP1 (563-767) in a ligand-dependent manner (Figure 8). However, in contrast to TR, extension of GRIP1 (563-767) to residue 1121 increases binding to GR about 3-fold suggesting an additional binding site on GRIP1 for GR. Binding of the larger fragment remains ligand-dependent; no interaction can be observed in the presence of the GR partial antagonist RU486. These results are in agreement with *in vivo* 2-hybrid GR GRIP1 interaction studies. In the presence of ligand no difference was detected in the binding of GRIP1 by full length GR or a deletion mutant of GR that lacks the N-terminal activation domain AF-1. However in the absence of ligand, binding of GR to GRIP1 (563-1121) increased by about 10-fold indicating that sequences in the GR N-terminus are able to suppress binding of unliganded GR to this additional binding site in GRIP1. Additionally, GR did not bind to a GRIP1 (563-767) mutant in which both NR-box 2 and 3 are replaced by alanines, and binds most strongly to a fragment that lacks a functional NR-box 2. As with TR, GR does not recognize NR-box 1. In contrast to TR, the GR prefers NR-box 3 to NR-box 2. These results demonstrate that GR prefers binding to NR-box 3 and interacts with an additional GRIP1 site within the CREB (cAMP - response - element binding protein) - binding protein (CBP) binding site.

Example 12: Coactivator peptide binding affinity for TR

- To investigate whether the preference of TR for NR-box 2 is dependent on the sequence or structural context of the NR-boxes, competition studies on the interaction of GRIP1 with hTR β LBD were performed using coactivator peptides containing different NR-boxes (NR-box 2 peptide (residues 11-23 of SEQ ID NO: 6) EKHKILHRLQLDS, and NR-box 3 peptide (residues 9-21 of SEQ ID NO: 7) ENALLRYLLDKDD) (Figure 9). Consistent with the interaction of hTR LBD β with GRIP1 (563-767) NR-box mutants, a peptide containing NR-box 1 competes the interaction of GRIP1 with hTR β LBD only at very high concentrations (EC_{50} = 130 μ M). Peptides containing either NR-box 2 or 3 compete GRIP1 (563-767) efficiently and display the preference of hTR β LBD for NR-box 2 (EC_{50} (NR-box 2) = 1.5 μ M, EC_{50} (NR-box 3) = 4 μ M). The apparent affinities (EC_{50}) for peptides of NR-box 2 and 3 are comparable with the analogous GRIP1 (563-767) NR-box mutants suggesting that the preference of TR for NR-boxes is solely dependent on the sequence and independent of the structural context of the NR-boxes.

5 Peptides of NR-box 2 or 3 compete GRIP1 (563-767) containing functional NR-boxes 2 and 3 or a mutant of this fragment that contains only a functional NR-box 2 with comparable affinity. Thus, while TR can bind both NR-box 2 and 3, in a GRIP1 coactivator peptide fragment containing both boxes, TR preferentially binds NR-box 2.

These results show the preference of TR for NR-box 2 is sequence dependent.

10 The same types of assays for TR competition are performed to assess coactivator peptide binding affinity for GR. The peptide concentrations are normalized relative to TR for obtaining comparable dose response curves.

Example 13: Binding affinity of TR for extended coactivator peptides

Sequence identity between all three central NR-boxes of the p160 coactivator family is
15 limited to the conserved leucine residues of the (SEQ ID NO: 1) LxxLL motif (Figure 6). However, the sequence conservation of a particular NR-box can extend into neighboring residues. To investigate the contribution of these neighboring residues to affinity and specificity of the different NR-boxes for TR, the ability of peptides containing individual NR-boxes with different lengths of adjacent sequences to compete with the interaction of GRIP1 (563-767) with hTRB LBD
20 were compared (Figure 10).

A peptide consisting of the minimal motif of NR-box 3 (residues 12-17 of SEQ ID NO: 7; LLRYLL) does not compete the TR LBD interaction with GRIP1 (563-767). A peptide consisting of the NR-box 2 (residues 15-20 of SEQ ID NO: 6; ILHRLL) also does not sufficiently compete the interaction (data not shown). Extending peptides containing a (SEQ ID NO: 1) LxxLL motif to
25 include adjacent residues increased affinity for both NR-box motifs and magnified the preference of TR for NR-box 2 (NR-box 2 peptides: (residues 11-23 SEQ ID NO: 6) EKHKILHRLLQDS and (residues 7-23 of SEQ ID NO: 6) TSLKEKHKILHRLLQDS; and NR-box 3 peptides: (residues 8-24 of SEQ ID NO: 7) KENALLRYLLDKDDTKD and (residues 5-24 of SEQ ID NO: 7) PKKKENALLRYLLDKDDTKD). A chimeric peptide containing the NR-box 3 motif in the
30 context of the NR-box 2 flanking sequences (SEQ ID NO: 31; TSLKEKHKLLRYLLQDSS) binds like a NR-box 2 peptide.

These results demonstrates that preference of TR for NR-box 2 is at least partially due to features of the bound peptide (residues 15-20 of SEQ ID NO: 6; ILHRLL), but that their affinity and specificity is modulated by adjacent sequences.

5 **Example 14: Binding affinity of TR and GR for mutant coactivator**

A. TR affinity for ILxxLL motif residues

To investigate the role of the hydrophobic residues in NR-box 2, individual residues of the (residues 15-20 of SEQ ID NO: 6) ILHRLL motif were replaced by alanine in the background of GRIP1 (563-767) containing a non-functional NR-box 3 (**Figure 11**). Surprisingly, replacement of
10 any of the conserved leucines prevents binding to TR almost completely. Only replacement of the nonconserved isoleucine exhibited a lessened but still severe impact on the affinity of NR-box 2 for TR. As replacement of a single leucine by alanine is sufficient to overcome the interaction of both the remaining hydrophobic residues and adjacent sequences with hTR β LBD, it appears that their contribution to the affinity of NR-box 2 for hTR β LBD is cooperative rather than additive.

15 Similar results were obtained by competing the interaction of hTR β LBD with the GRIP1 (563-767) NR-box 3 mutant using peptides in which either IL, HR or LL of the NR-box 2 motif are replaced by alanines (**Figure 11**). Whereas the peptides containing the IL or LL replacement failed to interact with the hTR β LBD even at very high concentrations, in agreement with a proposed alpha-helical structure of the motif, replacement of the "HR spacer" by alanines showed a marginal
20 effect on the affinity of the peptide for TR-LBD.

Replacement of single leucine residues of NR-box 2 by phenylalanine reduced the affinity of NR-box 2 peptides for TR LBD about 100-fold, replacement of the isoleucine about 10-fold (**Figure 11**). Therefore, the interaction of TR with GRIP1 relies not simply on the hydrophobicity of the (SEQ ID NO: 1) LxxLL motif, but also on positive contributions by the leucine residues
25 themselves.

These results demonstrate that single mutations of the conserved leucines in the (SEQ ID NO: 1) LxxLL motif strongly reduce affinity of GRIP1 for hTR β LBD.

Collectively, the above examples demonstrate that peptides containing NR-boxes, particularly NR-box 2, reproduce the affinity and specificity of the interaction of GRIP1 (563-767)
30 with hTR β LBD.

B. TR affinity of FxxLW and FxxAL motif residues

The three conserved leucines of the NR-box 2 (SEQ ID NO: 2) ILxxLL motif are embedded in the hydrophobic cleft of the hTR β LBD:NR-box 2 interaction surface, whereas the non conserved

5 isoleucine is located on the rim of this cleft where structural changes can be more easily accommodated (See Example 18). In agreement with this structure, replacement of this residue by alanine or phenylalanine reduced binding to hTR β LBD to a less extent than the comparable mutations of the conserved leucine residues. The surface generated by the three conserved leucines (L690, L693, L694) of the NR-box 2 peptide (residues 12-24 of SEQ ID NO: 6) 686-
10 KHKILHRLQLDSS-698 is highly complementary to the corresponding binding site in the hTR β LBD (Figures 16 and 17). Comparison of this binding site to other nuclear receptors shows that it contains a structural motif that is unique, highly conserved and present in all known structures of nuclear receptor LBDs (Wurtz et al., *Nat Struct Biol.* (1996) 3:87-94; Wagner et al., *supra*; Renaud et al., *Nature* (1995) 378:681-689; Bourguet et al., *Nature* (1995) 375:377-382; and Brzozowski et al., *Nature* (1997) 389:753-758).
15

Interaction of highly conserved hydrophobic motifs, which are part of amphipathic α -helices, with complementary hydrophobic surfaces resembles a feature observed for the interaction of several other transcriptional activators with their target proteins (p53:MDM2, VP16:TAFII31 or CREB:KIX-CBP). However, the motifs of p53 (FxxLW), VP16 (FxxAL) and CREB (YxxIL)
20 differ from the (SEQ ID NO: 1) LxxLL motif of nuclear receptor coactivators. A Fxxxh motif may be generally involved in interaction with TAFII31, where "h" represents any hydrophobic residue. Though with respect to the known structures, complementarity of the interacting hydrophobic surfaces identified here seem to be a common feature of these interactions, cross-reactions between different motifs are possible. For instance, VP16, p53, and p65 (FxxFL) are able to functionally
25 interact with TAFII31, or p53 and E2F1-DP1 (FxxLL) both interact with MDM2. These interactions are sensitive to mutations in the Fxxxh motif. Therefore it appears that either complementarity of the hydrophobic surfaces is not an absolute requirement or that induced fitting of the interacting surfaces is possible.

Based on these observations, studies were performed to determine whether GRIP1 interacts
30 with TAFII31 or MDM2. However, no interaction was detected. GRIP1 mutants changing NR-box 2 (SEQ ID NO: 1; LxxLL) to VP16 (SEQ ID NO: 4; FxxAL) or p53 (SEQ ID NO: 3; FxxLW) like binding sites also failed to bind TAFII31 or MDM2 demonstrating that the presence of the correct binding site is not sufficient to create binding (data not shown). Moreover, peptides containing the VP16 or p53 binding sites are not able to compete the interaction of GRIP1 with TR, even in very
35 high concentration, but do compete the interaction with GR (data not shown). The affinity of this interaction is weak, but comparable to affinity of a peptide of NR-box 2 that, in the context of a

- 5 GRIP1 mutant lacking NR-box 3, binds GR *in vivo* (Ding et al., *supra*). This binding is only about ten times less than a peptide containing NR-box 3, GR's primary binding site.

As shown above, GR binds GRIP1 (563-767) with about one-fifth the affinity than a comparable amount of TR. Thus, the high concentration of NR-box 3 peptide required to compete the interaction of GR with GRIP1 (563-767) may rather reflect a weak affinity of GR for the
10 peptide rather than a particular strong interaction of GR with GRIP1 (563-767).

These results suggest that at least on the peptide level, other hydrophobic motifs besides (SEQ ID NO: 1) LxxLL can interact with the coactivator binding site, but that it is receptor dependent.

C. TR affinity for residues adjacent to ILxxLL motif

- 15 Peptides containing a FxxLL motif bind TR but with two orders of magnitude lower affinity than a (SEQ ID NO: 1) LxxLL motif (**Figure 11**). To test whether the additional changes in the hydrophobic motif or adjacent sequences of the VP16 peptide prevent its binding to TR, a chimeric peptide containing the NR box-2 motif (SEQ ID NO: 1) LxxLL in the context of the VP16 sequence was constructed. This peptide binds to TR but with an about 100-fold lower affinity than the
20 original NR-box 2 peptide. Thus, the inability to bind the VP16 peptide appears to be due to the combination of an imperfect hydrophobic motif and the incompatibility of TR to adjacent sequences of the VP16 motif.

As the interaction of the chimeric peptide with GR was comparable to the original NR-box 2 and VP16 peptides, this incompatibility appears due to TR-specific features in the NR-box
25 interaction surface. These results show sequences adjacent the NR-box motif LxxLL can reduce binding of NR-box 2 to TR, but not GR.

Example 15: Crystallization and Structure Determination of NR LBD Complexes

A. Crystallization of hTR β LBD with T₃ and GRIP1 NR-box 2 Peptide

- Several peptides containing GRIP1 NR-box 2 were tested in crystallization trials with the
30 hTR β LBD. The complex of the hTR β LBD with the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) produced crystals that were dependent on both the presence and the concentration of the peptide. Without the peptide, the hTR β LBD precipitated immediately. However, nucleation was erratic, but could be overcome through seeding

5 of prepared drops with microcrystals of the hTR β LBD:GRIP1 NR-box 2 peptide complex. Structure of the hTR β LBD:GRIP1 NR-box 2 peptide complex was determined by molecular replacement using the structure of the hTR β LBD determined previously (Wagner et al., *supra*), and refined to a resolution of 3.6Å (Table 1). The refined model consists of residues K211-P254 and V264-D461 of monomer 1 of the hTR β LBD, residues K211-P254 and G261-D461 of monomer 2
10 of the hTR β LBD, and the GRIP1 NR-box 2 peptides (residues 14-24 of SEQ ID NO: 6) 688-KILHRLQLDSS-698, and (residues 14-22 of SEQ ID NO: 6) 688-KILHRLQLD-696 (Appendix 1).

Briefly, the complex between the hTR β LBD and the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) was prepared by mixing (equal)
15 volumes of a solution of 9mg/ml hTR β LBD in 20mM HEPES pH 7.4 with a solution of 14 mM GRIP1 in 0.4mM ammonium acetate pH 4.72, and incubating the mixture on ice for 1 hour. Crystals were obtained after 2 days at 4°C using hanging drop vapor diffusion from a drop containing 1.5µl of hTR β LBD:GRIP1 complex, prepared as described, and 0.5µl 15%PEG 4K, 0.2M sodium citrate pH 4.9, suspended above a reservoir containing 10% PEG 4K, 0.1M
20 ammonium acetate, and 0.05 M sodium citrate (pH 5.6). After allowing the drop to equilibrate for 1 hour, 0.2µl of 10⁻³ to 10⁻⁵ dilutions of microcrystals in reservoir buffer were introduced to provide nucleation. Crystals are of space group P3121 (a=95.2, b=95.2, c=137.6) and contain two molecules of the hTR β LBD and two molecules of the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6).

5

Table 1
Data collection, phasing, and refinement statistics

| Data collection | | | | | | |
|--------------------|------------------|------------------------|----------------|----------------|-------------------------|------------------------|
| Data set | Resolution (Å) | | Reflections | | Coverage (%) | R _{sym} |
| Native | 3.6 | | measured | unique | 96.3 | 0.007 |
| | | | 35565 | 8490 | | |
| Rotation search | | | | | | |
| Search model | Euler angles (°) | | | | Correlation coefficient | |
| | | Θ ₁ | Θ ₂ | Θ ₃ | Highest peak | Highest false peak |
| | hTR β LBD | M1 | 60.12 | 80.68 | 241.90 | 16.3 |
| | M2 | 9.93 | 87.70 | 180.6 | 15.9 | 14.2 |
| Translation search | | | | | | |
| | | Fractional coordinates | | | Translation function | |
| | | x | y | z | Highest peak (o) | Highest false peak (o) |
| | M1 | 0.522 | 0.428 | 0.250 | 19.52 | 10.02 |
| | M2 | 0.200 | 0.932 | 0.119 | 26.11 | 5.77 |
| Refinement | | | | | | |
| | Resolution (Å) | | Reflection | | R | R _{free} |
| F > 2(| 25 - 3.7 | | 7614 | | 0.2990 | 0.3219 |
| All data | 25 - 3.7 | | 7851 | | 0.3010 | 0.317 |

$R_{\text{sym}} = \sum_h \sum_i |I_{h,i} - \bar{I}_h| / \sum_h I_h$ for the intensity (I) of i observations of reflection h .

Correlation coefficient = $\sum_h E_o^2 E_c^2 - E_o^2 E_c^2 / [\sum_h (E_o^2 - E_o^2)^2 \sum_h (E_c^2 - E_c^2)^2]^{1/2}$

Translation function (t_a, t_b, \dots) = $\sum_h (|E_o(h)|^2 - \sum_h \langle |E_o(h)|^2 \rangle) (E_c(h, t_a, t_b, \dots))^2 - \langle |E_c(h)|^2 \rangle$

where E_o represents the normalized observed structure factor amplitudes, and E_c represents the normalized structure factors for the search model in a triclinic unit cell with dimensions identical to that of the crystal. The reported peak height represents the value of the function for the translation (t_a, t_b) of the NCS monomers, divided by the rms value of the translation function density.

R factor = $\sum |F_{\text{obs}} - F_{\text{calc}}| / \sum |F_{\text{obs}}|$.

R_{free} is calculated the same as R factor, except only for 10% of the reflections that were set aside for cross validation and not used in refinement.

5 **B. Crystallization of hER α LBD with DES and GRIP1 NR-box 2 Peptide**

Crystals of a DES-hER α LBD-GRIP1 NR-box 2 peptide complex were obtained by hanging drop vapor diffusion. Prior to crystallization, the DES-hER α LBD (residues 297-554) complex was incubated with a 2-4 fold molar excess of the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) for 7-16 hr. Two μ L samples of this solution were mixed
10 with equal volume samples of reservoir buffer consisting of 25-27% (w/v) PEG 4000, 90 mM Tris (pH 8.75-9.0) and 180 mM Na Acetate and suspended over wells containing 800 μ L of the reservoir buffer. After 4-7 days at 19-21°C, rod-like crystals were obtained. The coactivator complex crystals lie in the spacegroup P2₁ with cell dimensions a=54.09, b=82.22, c=58.04 and β =111.34. Two molecules each of the DES-LBD and the coactivator peptide form the asymmetric unit. A 200
15 μ m x 40 μ m x 40 μ m crystal was transferred to a cryosolvent solution containing 25% (w/v) PEG 4000, 10% (w/v) ethylene glycol, 100 mM Tris (pH 8.5), 200 mM Na Acetate and 10 μ M peptide and frozen in an N₂ stream at -170°C in a rayon loop. Diffraction data from this crystal were measured at -170°C using a 300 mm MAR image plate at the Stanford Synchrotron Radiation Laboratory (SSRL) at beamline 7-1 at a wavelength of 1.08 Å. The diffraction images were
20 processed with DENZO and scaled with SCALEPACK (Otwinowski, et al., *Methods Enzymol.* (1997) 276:307-326) using the default -3 σ cutoff.

C. Crystallization of hER α LBD with OHT

Crystals of the hER α LBD (residues 297-554) complexed to OHT were obtained by the hanging drop vapor diffusion method. Equal volume aliquots (2 μ L) of a solution containing 3.9
25 mg/mL protein-ligand complex and the reservoir solution containing 9% (w/v) PEG 8000, 6% (w/v) ethylene glycol, 50 mM HEPES (pH 6.7) and 200 mM NaCl were mixed and suspended over 800 μ L of the reservoir solution. Hexagonal plate-like crystals formed after 4-7 days at 21-23°C. Both crystal size and quality were improved through microseeding techniques. These crystals belong to the space group P6₅22 with cell parameters a=b=58.24 Å and c=277.47 Å. The asymmetric unit
30 consists of a single hER α LBD monomer; the dimer axis lies along a crystallographic two-fold. A single crystal (400 μ m x 250 μ m x 40 μ m) was briefly incubated in a cryoprotectant solution consisting of 10% (w/v) PEG 8000, 25% (w/v) ethylene glycol, 50 mM HEPES (pH 7.0) and 200 mM NaCl and then flash frozen in liquid N₂ suspended in a rayon loop. Diffraction data were measured at -170°C using a 345 mm MAR image plate at SSRL at beamline 9-1 and at a

- 5 wavelength of 0.98 Å. The diffraction images were processed with DENZO and scaled with SCALEPACK (Otwinowski, et al., *supra*) using the default -3σ cutoff.

Example 16: Structure determination and refinement of NR LBD complexes

A. Structure of hTR β LBD with T₃ and GRIP1 NR-box 2 Peptide

- 10 Data were measured using Cu Ka radiation from an R-axis generator at 50 kV and 300 mA with a 0.3mm collimator and a Ni filter. Reflections were measured using an R-Axis II detector and integrated with Denzo, and equivalent reflections scaled using Scalepack (Otwinowski and Minor, "Processing of x-ray diffraction data collected in oscillation mode." In *Macromolecular Crystallography, Part A* (ed. C.W. Carter, Jr. and R.M. Sweet), pp. 307-326. Academic Press, New York, NY). Possible rotation function solutions were calculated using normalized amplitudes in
- 15 AMORE from a model of hTR β LBD with the ligand, T₃, omitted; translation function solutions were subsequently determined using TFFC for the two rotation solutions with the highest correlation coefficients. For two hTR β LBD molecules in the asymmetric unit, the calculated solvent content is 52%. After rigid body refinement of the two hTR β LBD molecules, electron density maps were calculated. Strong positive density present in both the anomalous and
- 20 conventional difference Fourier maps for the iodine atoms of the T₃ ligand confirmed the correctness of the solution. The iodine atoms for both T₃ ligands were modeled as a rigid body, and the structure refined with strict NCS symmetry using CNS. Both 2FoFc and FoFc electron density maps showed interpretable density, related by the NCS operator, near H12 of both molecules of the hTR β LBD. The electron density could be modeled as a short α -helix, and the observed side chain
- 25 density was used to tentatively assign the sequence and direction to the chain. The refined model consists of residues of the hTR β LBD, and peptide residues of the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6).

Atomic coordinates of the hTR β LBD:GRP1 site 2 peptide complex are attached as Appendix 1.

30 **B. Structure of hER α LBD with DES and GRIP1 NR-box 2 Peptide**

Initial efforts to determine the structure of the DES-hER α LBD-NR box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) complex utilized a low resolution (3.1 Å) data set (data not shown). A self-rotation search implemented with POLARRFN ("The CCP4

5 suite: programs for protein crystallography", *Acta Crystallogr.* (1994) D50:760-763) indicated the presence of a noncrystallographic dyad. The two LBDs in the asymmetric were located by molecular replacement in AMoRe (CCP4, 1994) using a partial polyalanine model of the human RAR γ LBD (Renaud, et al., *supra*) as the search probe ($R=58.2\%$, $CC=35.6\%$ after placement of both monomers). Given that the model at this point was both inaccurate (r.m.s.d. 1.7 \AA between
10 this model and the final model based on $C\alpha$ positions) and incomplete (accounting for only $\sim 45\%$ of the total scattering matter in the asymmetric unit), an aggressive density modification protocol was undertaken. Iterative cycles of two-fold NCS averaging in DM (CCP4, 1994) interspersed with model building in MOLOC (Muller, et al., *Bull. Soc. Chim. Belg.* (1988) 97:655-667) and model refinement in REFMAC (Murshudov, et al., *Acta Crystallogr.* (1997) D53:240-255) (using tight
15 NCS restraints) were used to quickly build a model of the LBD alone. For this procedure, MAMA (Kleywegt, et al., "Halloween...masks and bones. In From First Map to Final Model", Bailey, et al, eds., Warrington, England, SERC Daresbury Laboratory, 1994) was used for all mask manipulations and PHASES (Furey, et al., PA33 *Am. Cryst. Assoc. Mtg. Abstr.* (1990) 18:73) and the CCP4 suite (CCP4, 1994) were used for the generation of structure factors and the calculation of
20 weights.

However, although the DES-hER α LBD-NR complex model accounted for $\sim 90\%$ of the scattering matter in the asymmetric unit, refinement was being hampered by severe model bias. The high-resolution data set of the DES-hER α LBD-NR-box 2 peptide complex became available when the R_{free} of the OHT-hER α LBD model was $\sim 31\%$. Both monomers in the asymmetric unit of
25 the DES complex crystal were relocated using AMoRe and the incompletely refined OHT-hER α LBD model (with helix 12 and the loop between helices 11 and 12 removed) as the search model. The missing parts of the model were built and the rest of the model was corrected using MOLOC and two-fold averaged maps generated in DM. Initially, refinement was carried out with REFMAC using tight NCS restraints. At later stages, the model was refined without NCS restraints using the
30 simulated annealing, minimization and B-factor refinement protocols in X-PLOR and a maximum-likelihood target. All B-factors were refined isotropically and anisotropic scaling and a bulk solvent correction were used. The R_{free} set contained a random sample of 6.5% of all data. In refinement, all data between 27 and 2.03 \AA (with no σ cutoff) were used. The final model was composed of residues 305-549 of monomer A, residues 305-461 and 470-554 of monomer B, residues 687-697 of
35 peptide A, residues 686-696 of peptide B, 164 waters, two carboxymethyl groups and a chloride ion. According to PROCHECK, 93.7% of all residues in the model were in the core regions of the Ramachandran plot and none were in the disallowed regions. Thus, the structure of the DES-hER α

5 LBD-NR-box 2 peptide complex has been refined to a crystallographic R-factor of 19.9% ($R_{\text{free}}=25.0\%$) using data to 2.03 Å resolution.

Ile 689 from the peptide interacts with three receptor residues (Asp 538, Glu 542 and Leu 539). The γ -carboxylate of Glu 542 forms hydrogen bonds to the amides of residues 689 and 690 of the peptide. A water-mediated hydrogen bond network is formed between the imidazole ring of His 10 377, the γ -carboxylate of Glu 380, and the amide of Tyr 537. Three residues (Glu 380, Leu 536 and Tyr 537) interact with each other through van der Waals contacts and/or hydrogen bonds. Intriguingly, mutations in each these three residues dramatically increase the transcription activity of unliganded ER α LBD (Eng, et al., *Mol. Cell. Biol.* (1997) 17:4644-4653); Lazennec, et al., *Mol. Endocrinol.* (1997) 11:1375-86; White, et al., *EMBO J.* (1997) 16:1427-35). Atomic coordinates of 15 DES-LBD-peptide complex are attached as **Appendix 2**.

5

Table 2

Summary of Crystallographic Statistics

| | <u>Data Collection</u> | <u>Ligand</u> | |
|----|--|-----------------|--------------------|
| | | <u>DES</u> | <u>OHT</u> |
| 10 | Space group | P2 ₁ | P6 ₅ 22 |
| | Resolution | 2.03 | 1.90 |
| | Observations | 104189 | 269253 |
| | Unique | 30265 | 23064 |
| | Completeness (%) | 98.4 | 99.1 |
| | R _{sym} (%) ^a | 7.8 | 7.0 |
| 15 | Average I/σI | 9.8 | 16.1 |
| | <u>Refinement</u> | | |
| | Number of non-hydrogen atoms | 4180 | 2070 |
| 20 | R _{cryst} (%) ^b /R _{free} (%) | 19.9/25.0 | 23.0/26.1 |
| | Bond r.m.s. deviation (Å) | 0.006 | 0.006 |
| | Angle r.m.s. deviation (°) | 1.05 | 1.05 |
| | Average B factor (Å ²) | 34.0 | 40.4 |
| | ^a R _{sym} = Σ _i I _i - <I> / Σ _i I _i where <I> is the average intensity over symmetry equivalents | | |
| 25 | ^b R _{cryst} = Σ F _o - F _c / Σ F _o | | |

C. Structure of hERα LBD-OHT complex

30 The OHT complex data set was then collected. Starting with one of the monomers of the preliminary low-resolution DES-hERα LBD-NR-box 2 peptide model as the search probe, molecular replacement in AMoRe was used to search for the location of LBD in this crystal form in both P6₁22 and P6₅22. A translation search in P6₅22 yielded the correct solution (R=53.8%, CC=38.2%). In order to reduce model bias, DMMULTI (CCP4, 1994) was then used to project averaged density from the DES complex cell into the OHT complex cell. Using MOLOC, a model of the hERα LBD was built into the resulting density. The model was refined initially in REFMAC and later with the simulated annealing, positional and B-factor refinement protocols in X-PLOR

5 (Brunger, X-PLOR Version 3.843, New Haven, Connecticut: Yale University, 1996) using a maximum-likelihood target (Adams, et al., *Proc. Natl. Acad. Sci. USA* (1997) 94:5018-23). Anisotropic scaling and a bulk solvent correction were used and all B-factors were refined isotropically. Except for the R_{free} set (a random sampling consisting of 8% of the data set), all data between 41 and 1.9 Å (with no σ cutoff) were included. The final model consisted of residues 306-10 551, the ligand and 78 waters. According to PROCHECK (CCP4, 1994), 91.6% of all residues in the model were in the core regions of the Ramachandran plot and none were in the disallowed regions. Thus, the structure of the OHT-hER α LBD complex has been refined against data of comparable resolution (1.90 Å) to a crystallographic R-factor of 23.0% (R_{free} =26.2%). Atomic coordinates of OHT-hER α LBD complex are attached as Appendix 3.

15 Example 17: Structural analysis of hTR β LBD:GRIP 1 NR-box 2 peptide complex

A. Structure of cocrystal complex (contents of asu)

The asymmetric unit (asu) of the crystal contains two monomers of the hTR β LBD and two molecules of the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6), which observes the NCS relation of the two TR monomers (Figure 12). The structure 20 of the hTR β LBD, which closely resembles that of the rTR α LBD (Wagner et al., *supra*), consists of twelve alpha-helices and two β -strands organized in three layers, resembling an alpha-helical sandwich. The only significant difference between the hTR β LBD and the rTR α LBD is disorder in the loop between helices H1 and H3. The GRIP1 NR-box 2 peptide forms an amphipathic α -helix of about 3 turns, preceded by 2 residues and followed by 3 residues in extended coil conformation.

25 The relation of the two monomers of the hTR β LBD is primarily translational, and does not resemble the homodimer structures reported for the hRXR, or the hER (Bourguet et al., *supra*; Brzozowski et al., *supra*). Furthermore, the interface between the two monomers does not involve residues necessary for formation of the physiological TR dimer. Instead, one of the cocrystal peptides appears to bridge the interaction between the two monomers. The hydrophobic face of the 30 alpha-helix of the cocrystal peptide contacts monomer 1 of the hTR β LBD at H3, H5, and H12, while the hydrophilic face contacts monomer 2 at the hairpin turn preceding strand S3. The second cocrystal peptide also contacts monomer 2 at H3, H5, and H12, and the two cocrystal peptides observe the same NCS relation as TR LBD monomers.

5 The common interface between both cocrystal peptides and the hTR β LBD buries the hydrophobic residues that define the cocrystal peptide (SEQ ID NO: 1) LxxLL sequence motif, residues Ile689, Leu690, Leu693, and Leu694; against the surface of the receptor LBD (Figures 16 and 17). The presence of the second peptide in the crystal, duplicating the interactions of the hydrophobic residues, suggests those interactions are specific and drive the interaction of the peptide with the hTR β LBD, while the hydrophilic interactions provide a fortuitous crystal contact and account for the dependence of crystallization on the presence and concentration of the peptide.

B. Structure of the GRIP1 NR-box 2 peptide

15 The GRIP1 NR-box 2 peptide used in the crystallization is 13 amino acids long (residues 12-24 of SEQ ID NO: 6; 686-KHKILHRLQLDSS-698). For the NR-box 2 peptide in monomer 1 (peptide 1), 12 amino acids are ordered in the crystal. Residues K688 - Q694 form an amphipathic helix, with residues K686-H687 and D695-S698 on either end in extended coil conformations. For the NR-box 2 peptide in monomer 2 (peptide 2), residues K688 - Q694 again form an amphipathic helix, but the ends of the peptide are disordered. While the resolution of the current data prevents absolute assignment of hydrogen bonds, it is evident from the periodicity of the side chain density that the central residues form an alpha-helix. In the absence of TR the far UV-CD spectrum of the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) appears to be random coil (data not shown). Stable helix formation may thus be induced by the interaction of the hydrophobic amino acids with the receptor LBD as it has been proposed in other protein:protein interactions, such as p53:MDM2 (Kussie et al., *Science* (1996) 274:948-953), VP16:TAF31 (Uesugi et al., *Science* (1996) 277:1310-1313), and CREB:KIX-CBP (Radhakrishnan et al., *Cell* (1997) 91:741-752).

C. Structure of the hTR β LBD:GRIP1 NR-box 2 peptide interface

30 The hTR β LBD of the cocrystal contributes residues from three helices, H3, H5, and H12 to the interface, which pack against one another to create a hydrophobic cleft. The residues lining the cleft are I280, T281, V283, V284, A287, and K288 from H3; Q301, I302, L305, and K306 from H5; and L454, E457, V458, and F459 from H12. A cysteine residue (C309) from H6 appears to provide a partial surface that is buried deep within the bottom of the cleft.

The GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) binds at the junction of H3 and H12. Leu690 of the bound peptide inserts into a shallow but

5 defined depression at the base of the cleft, making van der Waals contact with L454 and V458 of H12, while peptide residue Ile689 packs against L454 of H12 outside the edge of the cleft; L454, then, interdigitates between the two residues. One further turn C-terminal along the alpha-helix, L693 and L694 of the bound peptide pack into complementary pockets within the hydrophobic cleft. Peptide residue L693 forms van der Waals contact with V284 of H3, while peptide residue
10 L694, bound more deeply in the cleft, makes contact with F298 and L305 of H4 and H5. The hydrophobic interactions of the GRIP1 NR-box 2 peptide with the hTR β LBD are observed for both cocrystal peptides 1 and 2 in their respective monomers of the crystal dimer complex, suggesting that the interactions are specific to the peptide, and not induced by crystallization.

Example 18: Overall Structure of the DES-hER α -LBD-NR-box 2 Peptide Complex

15 The asymmetric unit of the DES-hER α LBD-NR-box 2 peptide 686-KHKILHRLQLQDSS-698 (residues 12-24 of SEQ ID NO: 6) complex crystals contains the same noncrystallographic dimer of LBDs that has been observed in the previously determined structures of the LBD bound to both E₂ and RAL (Brzozowski, et al., *supra* and Tanenbaum, et al., *supra*). Beyond the flexible loops between helices 2 and 3 and helices 9 and 10, the two LBDs of the dimer adopt similar
20 structures (r.m.s.d. 0.47 Å based on C α positions). The conformation of each LBD complexed with DES closely resembles that of the LBD bound to E₂ (Brzozowski, et al., *supra*); each monomer is a wedge shaped molecule consisting of three layers of eleven to twelve helices and a single beta hairpin. In each LBD, the hydrophobic face of helix 12 is packed against helices 3, 5/6 and 11 covering the ligand binding pocket. One NR-box 2 peptide is bound to each LBD in a hydrophobic
25 cleft composed of residues from helices 3, 4, 5 and 12 and the turn between 3 and 4. The density for both peptides in the asymmetric unit is continuous and unambiguous. Residues 687 to 697 from peptide A and residues 686 to 696 from peptide B have been modeled; the remaining residues are disordered. Given that each peptide lies within a different environment within the crystal, it is striking that from residues Ile 689 to Gln 695 each peptide forms a two turn, amphipathic α helix.
30 Flanking this region of common secondary structure, the peptides adopt dissimilar random coil conformations.

Example 19: Structure of the OHT-hER α LBD Complex

The binding of OHT induces a conformation of the hER α LBD that differs in both secondary and tertiary structural organization from that driven by DES binding. In the DES

5 complex, the main chain from residues 339 to 341, 421 to 423, and 527 to 530 form parts of helices 3, 8 and 11 respectively. In contrast, these regions adopt an extended conformation in the OHT complex. In addition, the composition and orientation of helix 12 are different in the two structures. Helix 12 in the DES complex consists of residues 538 to 546 whereas helix 12 in the OHT complex consists of residues 536 to 544. Most dramatically, rather than covering the ligand binding pocket
10 as it does in the DES complex, helix 12 in the OHT complex occupies the part of the coactivator binding groove formed by residues from helices 3, 4, and 5, and the turn connecting helices 3 and 4. This alternative conformation of helix 12 appears to be similar to that observed in the RAL complex (Brzozowski, et al., *supra*).

Example 20: Coactivator binding site structure and function

15 A. TR coactivator binding site

The above examples demonstrate that nuclear receptors, exemplified by TR, GR and ER, are recognized by specific coactivators that bind thereto through a coupling surface comprising a hydrophobic cleft and a charged hydrophobic perimeter. Identification and characterization of this coupling surface and the coactivator binding site of nuclear receptors offers a new target for the
20 design and selection of compounds that modulate binding of coactivator to nuclear receptors.

Residues forming the coactivator binding site were found to cluster within a surprisingly small area with well-defined borders (see, e.g., **Figures 5, 14, and 15**). As is shown in above Examples, mutated residues nearby this area do not affect coactivator binding or transcriptional activation. Additionally, the coactivator binding assays and structural analyses demonstrated that
25 NR-box containing proteins and peptides bind to this site. These results also showed that the GRIP1 coactivator protein binds to the site through a highly (SEQ ID NO: 1) LxxLL.

The structural analyses showed that residues contacting a conserved leucine residue of the (SEQ ID NO: 1) LxxLL motif included V284, F293, I302, L305 and L454. Residues within 4.5Å of an atom of the bound peptide included T281, V284, K288, F293, Q301, I302, L305, K306, P453,
30 L454 and E457. Structural analyses also revealed two other features of the site: a hydrophobic residue from helix 12 (Phe459) that contributes to local packing, and a cysteine residue contributed by helix 6 (Cys309) that provides a partial surface buried deep within the site. Mutational analyses showed that residues which block GRIP1 and SRC-1 coactivator binding when mutated are residues V284, K288, I302, K306, L454, and V458. Mutated residues likely to undergo a conformational
35 change upon hormone binding included Leu454 and Glu457. Thus, the site identified by

5 mutational, binding assays and crystallography corresponds to a surprisingly small cluster of residues on the surface of the LBD that define a prominent hydrophobic cleft formed by hydrophobic residues corresponding to human TR residues of C-terminal helix 3 (Ile280, Val283, Val284, and Ala287), helix 4 (Phe293), helix 5 (Ile302 and Leu305), helix 6 (Cys309), and helix 12 (Leu454, Val458 and Phe459). Collectively, the Examples indicate that residues forming the site
10 are amino acids corresponding to human TR residues of C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459). The coactivator binding site is highly conserved among the nuclear receptor super family (Figure 19).

The coactivator binding site of TR contains charged and hydrophobic residues at its
15 periphery, but only hydrophobic residues at its center (see, e.g., Figures 5 and 18). The hydrophobic cleft at the center of the site may play a significant role in driving the coactivator binding reaction. The site is comprised of two parts (Figure 18), right). Residues contained in helices 3, 5 and 6 (Figure 18, yellow residues) likely form a constitutive part, since their positions are identical in all nuclear receptor structures reported, including the liganded, activated states of
20 the TR, RAR, and ER, the unliganded RXR, and the inhibitor-liganded ER. By contrast, the residues of helix 12 (Figure 18, red residues) are differently positioned in the active and inactive states reported. Thus the coactivator binding site for the nuclear receptors is likely to be formed in response to an active hormone by positioning helix 12 against a scaffold formed by helices 3-6. Because the coactivator binding site is so small, it is easy to understand how even slight changes in
25 the position of helix 12, which may, for example, be induced by an antagonist ligand, could impair coactivator binding, and thus receptor activation.

B. ER coactivator binding site

Binding of the NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) to the ER α LBD buries 1000 Å² of predominantly hydrophobic surface area from both
30 molecules. The NR-box 2 peptide binding site is a shallow groove composed of residues Leu 354, Val 355, Ile 358, Ala 361 and Lys 362 from helix 3; Phe 367 and Val 368 from helix 4; Leu 372 from the turn between helices 3 and 4; Gln 375, Val 376, Leu 379 and Glu 380 from helix 5; and Asp 538, Leu 539, Glu 542 and Met 543 from helix 12. The floor and sides of this groove are completely nonpolar, but the ends of this groove are charged. Therefore, structural characterization
35 of the binding site of the NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) to the ER α LBD, which is the same NR-box 2 peptide utilized to crystallize the T₃-TR

5 LBD, supports the findings for TR that residues forming the coactivator binding site of nuclear
receptors is composed of a well defined hydrophobic cleft and a charged hydrophobic perimeter.
These residues are highly conserved among the nuclear receptor super family (Figure 19).
Structural characterization of the coactivator peptide-bound ER LBD also supports the concept of
exploiting the slight differences among the coactivator binding sites of nuclear receptors in
10 designing and identifying compounds that target specific nuclear receptors.

The ER α LBD interacts primarily with the hydrophobic face of the NR-box 2 peptide 686-
KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) α helix formed by the side chains of
Ile 689 and the three (SEQ ID NO: 1) LxxLL motif leucines (Leu 690, Leu 693 and Leu 694). The
side chain of Leu 690 is deeply embedded within the groove and forms van der Waals contacts with
15 the side chains of Ile 358, Val 376, Leu 379, Glu 380 and Met 543. The side chain of Leu 694 is
similarly isolated within the groove and makes van der Waals contacts with the side chains of Ile
358, Lys 362, Leu 372, Gln 375, Val 376 and Leu 379. In contrast, the side chains of both Ile 689
and the second NR box leucine, Leu 693, rest against the rim of the groove. The side chain of Ile
689 lies in a shallow depression formed by the side chains of Asp 538, Leu 539 and Glu 542. The
20 side chain of Leu 693 makes nonpolar contacts with the side chains of Ile 358 and Leu 539.

The charged and polar side chains which form the hydrophilic face of the peptide helix
project away from the ER α receptor and either interact predominantly with solvent or form
symmetry contacts. None of the side chains of the polar and charged residues outside the helical
region of either peptide in the asymmetric unit, with the exception of Lys 688 of peptide B, is
25 involved in hydrogen bonds or salt bridges with its associated ER α LBD monomer. The ϵ -amino
group of Lys 688 of peptide B hydrogen bonds to the side chain carboxylate of Glu 380 of
monomer B. This interaction is presumably a crystal artifact; the main chain atoms of the N-
terminal three residues of peptide B are displaced from monomer B and interact extensively with a
symmetry-related ER α LBD.

30 In addition to interacting with the hydrophobic face of the peptide helix, the ER α LBD
stabilizes the main chain conformation of the NR box peptide by forming capping interactions with
both ends of the peptide helix. Glu 542 and Lys 362 are positioned at opposite ends of the peptide
binding site. The side chains of Glu 542 and Lys 362 form van der Waals contacts with main chain
and side chain atoms at the N- and C-terminal turns of the peptide helix respectively. These
35 interactions position the stabilizing charges of the γ -carboxylate of Glu 542 and ϵ -amino group of
Lys 362 near the ends of the NR box peptide helix. The side chain carboxylate of Glu 542

5 hydrogen bonds to the amides of the residues of N-terminal turn of the peptide helix (residues 688 and 689 of peptide A; residues 689 and 690 of peptide B). Similarly, the ϵ -amino group of Lys 362 hydrogen bonds to the carbonyls of the residues of the C-terminal turn of the peptide helix (residue 693 of peptide A; residues 693 and 694 of peptide B).

10 Except for the orientation of helix 12, the structure of the peptide binding groove of the ER α LBD is almost identical in the DES and OHT complexes. The region of this groove outside of helix 12 is referred to herein as the "static region" of the NR box binding site. Helix 12 in the OHT complex and the NR box peptide helix in the DES complex interact with the static region of the coactivator recognition groove in strikingly similar ways.

15 Helix 12 mimics the hydrophobic interactions of the NR box peptide with the static region of the groove with a stretch of residues (residues 540 to 544) that resembles an NR box ((residues 6-10 of SEQ ID NO: 43) LLEML instead of (SEQ ID NO: 1) LxxLL). The side chains of Leu 540 and Met 543 lie in approximately the same locations as those of the first and second motif leucines (Leu 690 and Leu 693) in the peptide complex. Leu 540 is inserted into the groove and makes van der Waals contacts with Leu 354, Val 376 and Glu 380. Met 543 lies along the edge of the groove
20 and forms van der Waals contacts with the side chains of Leu 354, Val 355 and Ile 358. The side chain position of Leu 544 almost exactly overlaps that of the third NR box leucine, Leu 694. Deep within the groove, the Leu 544 side chain makes van der Waals contacts with the side chains of Ile 358, Lys 362, Leu 372, Gln 375, Val 376 and Leu 379.

Helix 12 in the OHT complex is also stabilized by N- and C-terminal capping interactions.
25 Lys 362 interacts with the C-terminal turn of helix 12 much as it does with the equivalent turn of the peptide helix. The Lys 362 side chain packs against the C-terminal turn of the helix 12 with its ϵ -amino group hydrogen bonding to the carbonyls of residues 543 and 544. Given that the capping interaction at the N-terminal turn coactivator helix is formed by a helix 12 residue (Glu 542), the N-terminal turn of helix 12 in the antagonist complex is forced to interact with another residue, Glu
30 380. The Glu 380 γ -carboxylate forms van der Waals contacts with Tyr 537 and interacts with the amide of Tyr 537 through a series of water-mediated hydrogen bonds.

In addition to forming these "NR box-like" interactions, helix 12 also forms van der Waals contacts with areas of the ER α LBD outside of the coactivator recognition groove. The side chain of Leu 536 forms van der Waals contacts with Glu 380 and Trp 383 and that of Tyr 537 forms van
35 der Waals contacts with His 373, Val 376 and Glu 380. As a result of these contacts, helix 12 in the

- 5 OHT complex buries more solvent accessible surface area ($\sim 1200 \text{ \AA}^2$) than the NR box peptide in the DES-ER α LBD-peptide complex.

Identification and characterization of the coactivator binding site for TR, and extension of this information to other nuclear receptors shows that this site is common for all nuclear receptors identified to date. Additionally, sequence and structural comparison, coupled with the Examples
10 showing differential specificity for coactivator binding to TR, GR and ER, reveal that minor differences between the receptors, such as found in helix 12, are likely to influence specificity of a coactivator for different types of nuclear receptors. Thus, the Examples presented herein demonstrate that information derived from the structure and function of the TR coactivator binding site can be applied in design and selection of compounds that modulate binding of coactivator
15 proteins to nuclear receptors for all members of the nuclear receptor super family.

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All publications and patent applications mentioned in this specification are herein incorporated by reference to the same extent as if each individual publication or patent application was specifically and individually indicated to be incorporated by reference.

30 The invention now being fully described, it will be apparent to one of ordinary skill in the art that many changes and modifications can be made thereto without departing from the spirit or scope of the appended claims.

5

Appendix 1

Atomic Coordinates for Human TR- β Complexed With T₃, and a GRIP1 NR-box 2 Peptide

REMARK full length numbering
 10 REMARK all residue names correct
 REMARK peptide sequence
 REMARK two molecules of TRB - CHAIN A and CHAIN B
 REMARK two molecules of T3 - CHAIN J and CHAIN K
 REMARK two molecules of GRIP-1 peptide - CHAIN X and CHAIN Y
 15 REMARK chain X lies between A and B
 REMARK chain Y interacts with B only
 REMARK residues differing between A and B include:
 REMARK A 217 Glu, A 252 Gln, A 263 Lys (missing side chains)
 REMARK B 237 Ser, B239 His, B 394 Lys (missing side chains)
 20 REMARK additionally Gly 261, Gly 262 are not visible in chain A
 REMARK residues differing between X and Y include:
 REMARK A 692 Arg
 REMARK additionally, residues Lys 688, Lys 689; Ser 697, Ser 698
 REMARK are not visible in chain Y

| | | | | | | | | | | |
|----|------|----|-----|-----------|--------|--------|--------|------|-------|---|
| 25 | ATOM | 1 | N | LYS A 211 | 52.546 | 23.912 | 35.239 | 1.00 | 45.76 | 7 |
| | ATOM | 2 | CA | LYS A 211 | 52.944 | 24.345 | 36.586 | 1.00 | 43.42 | 6 |
| | ATOM | 3 | C | LYS A 211 | 52.035 | 23.665 | 37.836 | 1.00 | 35.68 | 6 |
| | ATOM | 4 | O | LYS A 211 | 51.511 | 22.556 | 37.763 | 1.00 | 33.58 | 8 |
| | ATOM | 5 | CB | LYS A 211 | 52.610 | 25.825 | 36.779 | 1.00 | 46.72 | 6 |
| 30 | ATOM | 6 | N | PRO A 212 | 51.678 | 24.182 | 39.199 | 1.00 | 35.64 | 7 |
| | ATOM | 7 | CD | PRO A 212 | 52.082 | 25.474 | 39.842 | 1.00 | 38.60 | 6 |
| | ATOM | 8 | CA | PRO A 212 | 50.809 | 23.379 | 40.166 | 1.00 | 38.35 | 6 |
| | ATOM | 9 | CB | PRO A 212 | 50.670 | 24.194 | 41.440 | 1.00 | 38.95 | 6 |
| | ATOM | 10 | CG | PRO A 212 | 51.455 | 25.469 | 41.255 | 1.00 | 42.00 | 6 |
| 35 | ATOM | 11 | C | PRO A 212 | 49.433 | 23.097 | 39.594 | 1.00 | 38.78 | 6 |
| | ATOM | 12 | O | PRO A 212 | 48.920 | 23.949 | 38.802 | 1.00 | 34.64 | 8 |
| | ATOM | 13 | N | GLU A 213 | 48.901 | 21.948 | 40.014 | 1.00 | 40.31 | 7 |
| | ATOM | 14 | CA | GLU A 213 | 47.609 | 21.419 | 39.529 | 1.00 | 43.87 | 6 |
| | ATOM | 15 | CB | GLU A 213 | 47.943 | 20.307 | 38.520 | 1.00 | 45.16 | 6 |
| 40 | ATOM | 16 | CG | GLU A 213 | 49.125 | 20.708 | 37.601 | 1.00 | 47.60 | 6 |
| | ATOM | 17 | CD | GLU A 213 | 49.284 | 19.828 | 36.353 | 1.00 | 50.68 | 6 |
| | ATOM | 18 | OE1 | GLU A 213 | 49.355 | 18.547 | 36.474 | 1.00 | 59.18 | 8 |
| | ATOM | 19 | OE2 | GLU A 213 | 49.356 | 20.368 | 35.180 | 1.00 | 49.06 | 8 |
| | ATOM | 20 | C | GLU A 213 | 46.711 | 20.988 | 40.747 | 1.00 | 45.96 | 6 |
| 45 | ATOM | 21 | O | GLU A 213 | 47.111 | 21.136 | 41.910 | 1.00 | 43.13 | 8 |
| | ATOM | 22 | N | PRO A 214 | 45.463 | 20.460 | 40.515 | 1.00 | 46.52 | 7 |
| | ATOM | 23 | CD | PRO A 214 | 44.985 | 20.184 | 39.148 | 1.00 | 46.44 | 6 |
| | ATOM | 24 | CA | PRO A 214 | 44.447 | 20.124 | 41.596 | 1.00 | 47.52 | 6 |
| | ATOM | 25 | CB | PRO A 214 | 43.249 | 19.629 | 40.816 | 1.00 | 45.40 | 6 |
| 50 | ATOM | 26 | CG | PRO A 214 | 43.588 | 19.674 | 39.327 | 1.00 | 49.89 | 6 |
| | ATOM | 27 | C | PRO A 214 | 44.787 | 19.082 | 42.625 | 1.00 | 45.70 | 6 |
| | ATOM | 28 | O | PRO A 214 | 45.816 | 18.466 | 42.535 | 1.00 | 44.49 | 8 |
| | ATOM | 29 | N | THR A 215 | 43.915 | 18.876 | 43.606 | 1.00 | 45.24 | 7 |
| | ATOM | 30 | CA | THR A 215 | 44.161 | 17.890 | 44.686 | 1.00 | 49.36 | 6 |
| 55 | ATOM | 31 | CB | THR A 215 | 44.163 | 18.586 | 46.093 | 1.00 | 44.86 | 6 |
| | ATOM | 32 | OG1 | THR A 215 | 42.878 | 18.447 | 46.728 | 1.00 | 52.26 | 8 |
| | ATOM | 33 | CG2 | THR A 215 | 44.514 | 20.031 | 45.974 | 1.00 | 39.43 | 6 |
| | ATOM | 34 | C | THR A 215 | 42.934 | 16.995 | 44.667 | 1.00 | 52.51 | 6 |

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|----|------|----|-----|-----------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 35 | O | THR A 215 | 41.816 | 17.501 | 44.691 | 1.00 | 53.48 | 8 |
| | ATOM | 36 | N | ASP A 216 | 43.118 | 15.683 | 44.607 | 1.00 | 58.81 | 7 |
| | ATOM | 37 | CA | ASP A 216 | 41.973 | 14.740 | 44.615 | 1.00 | 61.51 | 6 |
| | ATOM | 38 | CB | ASP A 216 | 42.386 | 13.451 | 45.343 | 1.00 | 70.57 | 6 |
| | ATOM | 39 | CG | ASP A 216 | 42.399 | 12.283 | 44.475 | 1.00 | 78.07 | 6 |
| 10 | ATOM | 40 | OD1 | ASP A 216 | 41.532 | 12.161 | 43.586 | 1.00 | 82.31 | 8 |
| | ATOM | 41 | OD2 | ASP A 216 | 43.293 | 11.436 | 44.684 | 1.00 | 86.55 | 8 |
| | ATOM | 42 | C | ASP A 216 | 40.640 | 15.311 | 45.268 | 1.00 | 58.42 | 6 |
| | ATOM | 43 | O | ASP A 216 | 39.598 | 14.840 | 44.924 | 1.00 | 56.85 | 8 |
| | ATOM | 44 | N | GLU A 217 | 40.673 | 16.270 | 46.217 | 1.00 | 54.92 | 7 |
| 15 | ATOM | 45 | CA | GLU A 217 | 39.502 | 16.937 | 46.856 | 1.00 | 53.37 | 6 |
| | ATOM | 46 | CB | GLU A 217 | 39.943 | 17.459 | 48.216 | 1.00 | 51.02 | 6 |
| | ATOM | 47 | C | GLU A 217 | 39.113 | 18.144 | 45.956 | 1.00 | 53.55 | 6 |
| | ATOM | 48 | O | GLU A 217 | 37.905 | 18.394 | 45.695 | 1.00 | 54.33 | 8 |
| | ATOM | 49 | N | GLU A 218 | 40.162 | 18.895 | 45.511 | 1.00 | 49.20 | 7 |
| 20 | ATOM | 50 | CA | GLU A 218 | 39.933 | 20.073 | 44.661 | 1.00 | 45.94 | 6 |
| | ATOM | 51 | CB | GLU A 218 | 41.232 | 20.855 | 44.304 | 1.00 | 43.43 | 6 |
| | ATOM | 52 | CG | GLU A 218 | 41.907 | 21.579 | 45.479 | 1.00 | 40.86 | 6 |
| | ATOM | 53 | CD | GLU A 218 | 43.061 | 22.446 | 45.074 | 1.00 | 39.88 | 6 |
| | ATOM | 54 | OE1 | GLU A 218 | 43.895 | 22.019 | 44.232 | 1.00 | 37.61 | 8 |
| 25 | ATOM | 55 | OE2 | GLU A 218 | 43.183 | 23.583 | 45.599 | 1.00 | 34.01 | 8 |
| | ATOM | 56 | C | GLU A 218 | 39.249 | 19.647 | 43.390 | 1.00 | 44.71 | 6 |
| | ATOM | 57 | O | GLU A 218 | 38.302 | 20.291 | 42.964 | 1.00 | 45.31 | 8 |
| | ATOM | 58 | N | TRP A 219 | 39.720 | 18.553 | 42.797 | 1.00 | 44.02 | 7 |
| | ATOM | 59 | CA | TRP A 219 | 39.109 | 18.061 | 41.574 | 1.00 | 46.97 | 6 |
| 30 | ATOM | 60 | CB | TRP A 219 | 39.799 | 16.793 | 41.074 | 1.00 | 48.42 | 6 |
| | ATOM | 61 | CG | TRP A 219 | 40.879 | 17.029 | 40.141 | 1.00 | 54.61 | 6 |
| | ATOM | 62 | CD2 | TRP A 219 | 40.755 | 17.256 | 38.733 | 1.00 | 55.24 | 6 |
| | ATOM | 63 | CE2 | TRP A 219 | 42.067 | 17.523 | 38.245 | 1.00 | 53.67 | 6 |
| | ATOM | 64 | CE3 | TRP A 219 | 39.691 | 17.234 | 37.828 | 1.00 | 54.55 | 6 |
| 35 | ATOM | 65 | CD1 | TRP A 219 | 42.159 | 17.159 | 40.447 | 1.00 | 55.75 | 6 |
| | ATOM | 66 | NE1 | TRP A 219 | 42.895 | 17.485 | 39.339 | 1.00 | 54.43 | 7 |
| | ATOM | 67 | CZ2 | TRP A 219 | 42.330 | 17.851 | 36.895 | 1.00 | 52.54 | 6 |
| | ATOM | 68 | CZ3 | TRP A 219 | 39.943 | 17.535 | 36.509 | 1.00 | 55.17 | 6 |
| | ATOM | 69 | CH2 | TRP A 219 | 41.239 | 17.820 | 36.029 | 1.00 | 55.59 | 6 |
| 40 | ATOM | 70 | C | TRP A 219 | 37.646 | 17.743 | 41.812 | 1.00 | 47.32 | 6 |
| | ATOM | 71 | O | TRP A 219 | 36.788 | 18.028 | 40.978 | 1.00 | 43.56 | 8 |
| | ATOM | 72 | N | GLU A 220 | 37.376 | 17.142 | 42.965 | 1.00 | 49.91 | 7 |
| | ATOM | 73 | CA | GLU A 220 | 36.021 | 16.769 | 43.316 | 1.00 | 53.57 | 6 |
| | ATOM | 74 | CB | GLU A 220 | 36.052 | 16.055 | 44.649 | 1.00 | 58.18 | 6 |
| 45 | ATOM | 75 | CG | GLU A 220 | 35.149 | 14.930 | 44.672 | 1.00 | 73.13 | 6 |
| | ATOM | 76 | CD | GLU A 220 | 35.735 | 13.935 | 45.442 | 1.00 | 80.06 | 6 |
| | ATOM | 77 | OE1 | GLU A 220 | 36.886 | 13.575 | 45.173 | 1.00 | 82.12 | 8 |
| | ATOM | 78 | OE2 | GLU A 220 | 35.078 | 13.478 | 46.378 | 1.00 | 82.78 | 8 |
| | ATOM | 79 | C | GLU A 220 | 35.161 | 18.026 | 43.381 | 1.00 | 50.51 | 6 |
| 50 | ATOM | 80 | O | GLU A 220 | 33.991 | 18.010 | 42.995 | 1.00 | 49.94 | 8 |
| | ATOM | 81 | N | LEU A 221 | 35.761 | 19.120 | 43.865 | 1.00 | 43.71 | 7 |
| | ATOM | 82 | CA | LEU A 221 | 35.047 | 20.398 | 43.951 | 1.00 | 42.81 | 6 |
| | ATOM | 83 | CB | LEU A 221 | 35.935 | 21.510 | 44.510 | 1.00 | 39.21 | 6 |
| | ATOM | 84 | CG | LEU A 221 | 35.375 | 22.908 | 44.353 | 1.00 | 36.34 | 6 |
| 55 | ATOM | 85 | CD1 | LEU A 221 | 33.941 | 22.929 | 44.836 | 1.00 | 36.93 | 6 |
| | ATOM | 86 | CD2 | LEU A 221 | 36.226 | 23.910 | 45.122 | 1.00 | 24.18 | 6 |
| | ATOM | 87 | C | LEU A 221 | 34.563 | 20.815 | 42.575 | 1.00 | 43.46 | 6 |
| | ATOM | 88 | O | LEU A 221 | 33.392 | 21.104 | 42.395 | 1.00 | 45.25 | 8 |

| | | | | | | | | | | | | |
|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 89 | N | ILE | A | 222 | 35.498 | 20.871 | 41.628 | 1.00 | 39.09 | 7 |
| | ATOM | 90 | CA | ILE | A | 222 | 35.192 | 21.226 | 40.254 | 1.00 | 35.47 | 6 |
| | ATOM | 91 | CB | ILE | A | 222 | 36.379 | 20.997 | 39.343 | 1.00 | 33.74 | 6 |
| | ATOM | 92 | CG2 | ILE | A | 222 | 35.970 | 21.182 | 37.893 | 1.00 | 28.86 | 6 |
| | ATOM | 93 | CG1 | ILE | A | 222 | 37.532 | 21.922 | 39.707 | 1.00 | 33.33 | 6 |
| 10 | ATOM | 94 | CD1 | ILE | A | 222 | 38.804 | 21.586 | 39.004 | 1.00 | 34.85 | 6 |
| | ATOM | 95 | C | ILE | A | 222 | 34.067 | 20.365 | 39.735 | 1.00 | 34.26 | 6 |
| | ATOM | 96 | O | ILE | A | 222 | 33.033 | 20.873 | 39.319 | 1.00 | 31.90 | 8 |
| | ATOM | 97 | N | LYS | A | 223 | 34.301 | 19.058 | 39.750 | 1.00 | 39.49 | 7 |
| | ATOM | 98 | CA | LYS | A | 223 | 33.316 | 18.100 | 39.276 | 1.00 | 44.43 | 6 |
| 15 | ATOM | 99 | CB | LYS | A | 223 | 33.603 | 16.713 | 39.852 | 1.00 | 50.81 | 6 |
| | ATOM | 100 | CG | LYS | A | 223 | 32.741 | 15.631 | 39.227 | 1.00 | 62.51 | 6 |
| | ATOM | 101 | CD | LYS | A | 223 | 32.859 | 14.291 | 39.943 | 1.00 | 72.22 | 6 |
| | ATOM | 102 | CE | LYS | A | 223 | 31.798 | 13.318 | 39.430 | 1.00 | 74.55 | 6 |
| | ATOM | 103 | NZ | LYS | A | 223 | 31.900 | 11.985 | 40.106 | 1.00 | 75.78 | 7 |
| 20 | ATOM | 104 | C | LYS | A | 223 | 31.913 | 18.565 | 39.681 | 1.00 | 42.81 | 6 |
| | ATOM | 105 | O | LYS | A | 223 | 30.936 | 18.323 | 38.984 | 1.00 | 40.36 | 8 |
| | ATOM | 106 | N | THR | A | 224 | 31.849 | 19.236 | 40.833 | 1.00 | 39.89 | 7 |
| | ATOM | 107 | CA | THR | A | 224 | 30.602 | 19.792 | 41.378 | 1.00 | 39.93 | 6 |
| | ATOM | 108 | CB | THR | A | 224 | 30.805 | 20.206 | 42.851 | 1.00 | 40.57 | 6 |
| 25 | ATOM | 109 | OG1 | THR | A | 224 | 31.330 | 19.113 | 43.616 | 1.00 | 39.27 | 8 |
| | ATOM | 110 | CG2 | THR | A | 224 | 29.500 | 20.684 | 43.461 | 1.00 | 38.11 | 6 |
| | ATOM | 111 | C | THR | A | 224 | 30.167 | 21.011 | 40.533 | 1.00 | 39.96 | 6 |
| | ATOM | 112 | O | THR | A | 224 | 29.313 | 20.899 | 39.655 | 1.00 | 36.67 | 8 |
| | ATOM | 113 | N | VAL | A | 225 | 30.777 | 22.160 | 40.832 | 1.00 | 38.02 | 7 |
| 30 | ATOM | 114 | CA | VAL | A | 225 | 30.532 | 23.426 | 40.137 | 1.00 | 38.12 | 6 |
| | ATOM | 115 | CB | VAL | A | 225 | 31.797 | 24.292 | 40.122 | 1.00 | 38.19 | 6 |
| | ATOM | 116 | CG1 | VAL | A | 225 | 31.512 | 25.636 | 39.491 | 1.00 | 36.77 | 6 |
| | ATOM | 117 | CG2 | VAL | A | 225 | 32.343 | 24.464 | 41.505 | 1.00 | 41.76 | 6 |
| | ATOM | 118 | C | VAL | A | 225 | 30.070 | 23.195 | 38.706 | 1.00 | 37.52 | 6 |
| 35 | ATOM | 119 | O | VAL | A | 225 | 29.119 | 23.803 | 38.239 | 1.00 | 36.77 | 8 |
| | ATOM | 120 | N | THR | A | 226 | 30.783 | 22.316 | 38.018 | 1.00 | 34.02 | 7 |
| | ATOM | 121 | CA | THR | A | 226 | 30.489 | 21.971 | 36.636 | 1.00 | 34.67 | 6 |
| | ATOM | 122 | CB | THR | A | 226 | 31.565 | 20.999 | 36.083 | 1.00 | 30.56 | 6 |
| | ATOM | 123 | OG1 | THR | A | 226 | 32.805 | 21.696 | 35.889 | 1.00 | 32.20 | 8 |
| 40 | ATOM | 124 | CG2 | THR | A | 226 | 31.108 | 20.346 | 34.783 | 1.00 | 20.99 | 6 |
| | ATOM | 125 | C | THR | A | 226 | 29.100 | 21.361 | 36.510 | 1.00 | 36.41 | 6 |
| | ATOM | 126 | O | THR | A | 226 | 28.255 | 21.877 | 35.785 | 1.00 | 39.64 | 8 |
| | ATOM | 127 | N | ALA | A | 227 | 28.880 | 20.260 | 37.222 | 1.00 | 39.20 | 7 |
| | ATOM | 128 | CA | ALA | A | 227 | 27.602 | 19.562 | 37.204 | 1.00 | 36.93 | 6 |
| 45 | ATOM | 129 | CB | ALA | A | 227 | 27.526 | 18.600 | 38.381 | 1.00 | 38.06 | 6 |
| | ATOM | 130 | C | ALA | A | 227 | 26.507 | 20.604 | 37.318 | 1.00 | 37.69 | 6 |
| | ATOM | 131 | O | ALA | A | 227 | 25.444 | 20.489 | 36.718 | 1.00 | 40.94 | 8 |
| | ATOM | 132 | N | ALA | A | 228 | 26.811 | 21.630 | 38.107 | 1.00 | 32.86 | 7 |
| | ATOM | 133 | CA | ALA | A | 228 | 25.903 | 22.734 | 38.356 | 1.00 | 32.48 | 6 |
| 50 | ATOM | 134 | CB | ALA | A | 228 | 26.448 | 23.587 | 39.486 | 1.00 | 28.25 | 6 |
| | ATOM | 135 | C | ALA | A | 228 | 25.732 | 23.570 | 37.101 | 1.00 | 36.12 | 6 |
| | ATOM | 136 | O | ALA | A | 228 | 24.673 | 23.560 | 36.473 | 1.00 | 37.86 | 8 |
| | ATOM | 137 | N | HIS | A | 229 | 26.782 | 24.306 | 36.752 | 1.00 | 33.58 | 7 |
| | ATOM | 138 | CA | HIS | A | 229 | 26.762 | 25.158 | 35.585 | 1.00 | 32.97 | 6 |
| 55 | ATOM | 139 | CB | HIS | A | 229 | 28.155 | 25.691 | 35.266 | 1.00 | 33.69 | 6 |
| | ATOM | 140 | CG | HIS | A | 229 | 28.250 | 26.333 | 33.929 | 1.00 | 28.39 | 6 |
| | ATOM | 141 | CD2 | HIS | A | 229 | 29.025 | 26.081 | 32.838 | 1.00 | 28.83 | 6 |
| | ATOM | 142 | ND1 | HIS | A | 229 | 27.386 | 27.368 | 33.542 | 1.00 | 30.47 | 7 |

| | | | | | | | | | | | | |
|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 143 | CE1 | HIS | A | 229 | 27.654 | 27.692 | 32.280 | 1.00 | 26.95 | 6 |
| | ATOM | 144 | NE2 | HIS | A | 229 | 28.635 | 26.934 | 31.840 | 1.00 | 31.27 | 7 |
| | ATOM | 145 | C | HIS | A | 229 | 26.225 | 24.541 | 34.312 | 1.00 | 38.40 | 6 |
| | ATOM | 146 | O | HIS | A | 229 | 25.591 | 25.227 | 33.528 | 1.00 | 41.49 | 8 |
| | ATOM | 147 | N | VAL | A | 230 | 26.519 | 23.256 | 34.113 | 1.00 | 38.55 | 7 |
| 10 | ATOM | 148 | CA | VAL | A | 230 | 26.088 | 22.554 | 32.916 | 1.00 | 40.40 | 6 |
| | ATOM | 149 | CB | VAL | A | 230 | 26.890 | 21.256 | 32.701 | 1.00 | 44.68 | 6 |
| | ATOM | 150 | CG1 | VAL | A | 230 | 26.557 | 20.656 | 31.345 | 1.00 | 39.39 | 6 |
| | ATOM | 151 | CG2 | VAL | A | 230 | 28.381 | 21.509 | 32.817 | 1.00 | 42.18 | 6 |
| | ATOM | 152 | C | VAL | A | 230 | 24.603 | 22.239 | 32.900 | 1.00 | 44.28 | 6 |
| 15 | ATOM | 153 | O | VAL | A | 230 | 23.959 | 22.316 | 31.847 | 1.00 | 45.94 | 8 |
| | ATOM | 154 | N | ALA | A | 231 | 24.072 | 21.862 | 34.059 | 1.00 | 45.59 | 7 |
| | ATOM | 155 | CA | ALA | A | 231 | 22.669 | 21.500 | 34.175 | 1.00 | 47.84 | 6 |
| | ATOM | 156 | CB | ALA | A | 231 | 22.482 | 20.582 | 35.374 | 1.00 | 45.08 | 6 |
| | ATOM | 157 | C | ALA | A | 231 | 21.792 | 22.734 | 34.314 | 1.00 | 48.04 | 6 |
| 20 | ATOM | 158 | O | ALA | A | 231 | 20.565 | 22.647 | 34.324 | 1.00 | 49.95 | 8 |
| | ATOM | 159 | N | THR | A | 232 | 22.436 | 23.894 | 34.384 | 1.00 | 47.26 | 7 |
| | ATOM | 160 | CA | THR | A | 232 | 21.722 | 25.161 | 34.528 | 1.00 | 43.64 | 6 |
| | ATOM | 161 | CB | THR | A | 232 | 22.112 | 25.832 | 35.850 | 1.00 | 41.93 | 6 |
| | ATOM | 162 | OG1 | THR | A | 232 | 23.467 | 26.283 | 35.791 | 1.00 | 39.10 | 8 |
| 25 | ATOM | 163 | CG2 | THR | A | 232 | 21.990 | 24.846 | 37.008 | 1.00 | 29.80 | 6 |
| | ATOM | 164 | C | THR | A | 232 | 22.055 | 26.114 | 33.387 | 1.00 | 43.97 | 6 |
| | ATOM | 165 | O | THR | A | 232 | 21.679 | 27.279 | 33.436 | 1.00 | 40.55 | 8 |
| | ATOM | 166 | N | ASN | A | 233 | 22.783 | 25.625 | 32.381 | 1.00 | 48.62 | 7 |
| | ATOM | 167 | CA | ASN | A | 233 | 23.134 | 26.468 | 31.231 | 1.00 | 58.62 | 6 |
| 30 | ATOM | 168 | CB | ASN | A | 233 | 24.626 | 26.283 | 30.880 | 1.00 | 62.44 | 6 |
| | ATOM | 169 | CG | ASN | A | 233 | 25.141 | 27.355 | 29.927 | 1.00 | 68.35 | 6 |
| | ATOM | 170 | OD1 | ASN | A | 233 | 24.822 | 28.544 | 30.096 | 1.00 | 65.50 | 8 |
| | ATOM | 171 | ND2 | ASN | A | 233 | 25.951 | 26.951 | 28.959 | 1.00 | 74.29 | 7 |
| | ATOM | 172 | C | ASN | A | 233 | 22.241 | 26.035 | 30.073 | 1.00 | 65.06 | 6 |
| 35 | ATOM | 173 | O | ASN | A | 233 | 22.312 | 24.900 | 29.604 | 1.00 | 69.47 | 8 |
| | ATOM | 174 | N | ALA | A | 234 | 21.381 | 26.954 | 29.646 | 1.00 | 68.80 | 7 |
| | ATOM | 175 | CA | ALA | A | 234 | 20.423 | 26.708 | 28.564 | 1.00 | 70.98 | 6 |
| | ATOM | 176 | CB | ALA | A | 234 | 19.748 | 28.015 | 28.186 | 1.00 | 71.43 | 6 |
| | ATOM | 177 | C | ALA | A | 234 | 20.988 | 26.062 | 27.308 | 1.00 | 73.83 | 6 |
| 40 | ATOM | 178 | O | ALA | A | 234 | 22.041 | 26.419 | 26.822 | 1.00 | 74.33 | 8 |
| | ATOM | 179 | N | GLN | A | 235 | 20.227 | 25.096 | 26.819 | 1.00 | 75.07 | 7 |
| | ATOM | 180 | CA | GLN | A | 235 | 20.562 | 24.363 | 25.629 | 1.00 | 76.32 | 6 |
| | ATOM | 181 | CB | GLN | A | 235 | 20.328 | 25.239 | 24.391 | 1.00 | 76.98 | 6 |
| | ATOM | 182 | CG | GLN | A | 235 | 18.887 | 25.292 | 23.908 | 1.00 | 77.07 | 6 |
| 45 | ATOM | 183 | CD | GLN | A | 235 | 17.896 | 25.420 | 25.019 | 1.00 | 80.85 | 6 |
| | ATOM | 184 | OE1 | GLN | A | 235 | 17.668 | 24.448 | 25.768 | 1.00 | 82.01 | 8 |
| | ATOM | 185 | NE2 | GLN | A | 235 | 17.313 | 26.596 | 25.149 | 1.00 | 78.80 | 7 |
| | ATOM | 186 | C | GLN | A | 235 | 21.960 | 23.840 | 25.573 | 1.00 | 77.15 | 6 |
| | ATOM | 187 | O | GLN | A | 235 | 22.386 | 23.458 | 24.508 | 1.00 | 76.06 | 8 |
| 50 | ATOM | 188 | N | GLY | A | 236 | 22.676 | 23.766 | 26.687 | 1.00 | 77.46 | 7 |
| | ATOM | 189 | CA | GLY | A | 236 | 24.053 | 23.245 | 26.627 | 1.00 | 78.37 | 6 |
| | ATOM | 190 | C | GLY | A | 236 | 24.923 | 23.491 | 25.390 | 1.00 | 79.43 | 6 |
| | ATOM | 191 | O | GLY | A | 236 | 24.917 | 24.565 | 24.844 | 1.00 | 79.47 | 8 |
| | ATOM | 192 | N | SER | A | 237 | 25.739 | 22.526 | 24.991 | 1.00 | 77.98 | 7 |
| 55 | ATOM | 193 | CA | SER | A | 237 | 26.566 | 22.760 | 23.801 | 1.00 | 76.49 | 6 |
| | ATOM | 194 | CB | SER | A | 237 | 27.981 | 22.206 | 24.015 | 1.00 | 76.46 | 6 |
| | ATOM | 195 | OG | SER | A | 237 | 28.821 | 23.145 | 24.689 | 1.00 | 40.00 | 8 |
| | ATOM | 196 | C | SER | A | 237 | 25.938 | 22.127 | 22.542 | 1.00 | 75.35 | 6 |

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|----|------|-----|-----|-------|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 197 | O | SER A | 237 | 26.605 | 21.418 | 21.797 | 1.00 | 75.47 | 8 |
| | ATOM | 198 | N | HIS A | 238 | 24.648 | 22.410 | 22.353 | 1.00 | 75.56 | 7 |
| | ATOM | 199 | CA | HIS A | 238 | 23.842 | 21.981 | 21.236 | 1.00 | 75.46 | 6 |
| | ATOM | 200 | CB | HIS A | 238 | 22.990 | 20.732 | 21.661 | 1.00 | 75.85 | 6 |
| | ATOM | 201 | CG | HIS A | 238 | 22.408 | 19.933 | 20.542 | 1.00 | 40.00 | 6 |
| 10 | ATOM | 202 | CD2 | HIS A | 238 | 22.790 | 18.757 | 19.957 | 1.00 | 40.00 | 6 |
| | ATOM | 203 | ND1 | HIS A | 238 | 21.223 | 20.303 | 19.875 | 1.00 | 40.00 | 7 |
| | ATOM | 204 | CE1 | HIS A | 238 | 20.951 | 19.365 | 18.953 | 1.00 | 40.00 | 6 |
| | ATOM | 205 | NE2 | HIS A | 238 | 21.874 | 18.444 | 18.994 | 1.00 | 40.00 | 7 |
| | ATOM | 206 | C | HIS A | 238 | 22.971 | 23.284 | 20.964 | 1.00 | 74.10 | 6 |
| 15 | ATOM | 207 | O | HIS A | 238 | 21.863 | 23.137 | 20.441 | 1.00 | 75.34 | 8 |
| | ATOM | 208 | N | TRP A | 239 | 23.487 | 24.510 | 21.368 | 1.00 | 73.39 | 7 |
| | ATOM | 209 | CA | TRP A | 239 | 22.872 | 25.894 | 21.195 | 1.00 | 74.02 | 6 |
| | ATOM | 210 | CB | TRP A | 239 | 23.563 | 27.026 | 22.005 | 1.00 | 81.77 | 6 |
| | ATOM | 211 | CG | TRP A | 239 | 25.022 | 27.366 | 21.688 | 1.00 | 89.67 | 6 |
| 20 | ATOM | 212 | CD2 | TRP A | 239 | 25.532 | 28.662 | 21.240 | 1.00 | 93.19 | 6 |
| | ATOM | 213 | CE2 | TRP A | 239 | 26.961 | 28.522 | 21.136 | 1.00 | 95.46 | 6 |
| | ATOM | 214 | CE3 | TRP A | 239 | 24.936 | 29.911 | 20.969 | 1.00 | 95.35 | 6 |
| | ATOM | 215 | CD1 | TRP A | 239 | 26.102 | 26.548 | 21.781 | 1.00 | 94.16 | 6 |
| | ATOM | 216 | NE1 | TRP A | 239 | 27.268 | 27.241 | 21.475 | 1.00 | 97.48 | 7 |
| 25 | ATOM | 217 | CZ2 | TRP A | 239 | 27.798 | 29.598 | 20.764 | 1.00 | 96.23 | 6 |
| | ATOM | 218 | CZ3 | TRP A | 239 | 25.763 | 30.967 | 20.569 | 1.00 | 96.75 | 6 |
| | ATOM | 219 | CH2 | TRP A | 239 | 27.171 | 30.825 | 20.482 | 1.00 | 97.32 | 6 |
| | ATOM | 220 | C | TRP A | 239 | 22.799 | 26.407 | 19.774 | 1.00 | 70.77 | 6 |
| | ATOM | 221 | O | TRP A | 239 | 21.706 | 26.562 | 19.263 | 1.00 | 71.70 | 8 |
| 30 | ATOM | 222 | N | LYS A | 240 | 23.946 | 26.701 | 19.157 | 1.00 | 67.10 | 7 |
| | ATOM | 223 | CA | LYS A | 240 | 23.978 | 27.180 | 17.783 | 1.00 | 65.63 | 6 |
| | ATOM | 224 | CB | LYS A | 240 | 25.314 | 26.780 | 17.153 | 1.00 | 66.65 | 6 |
| | ATOM | 225 | CG | LYS A | 240 | 26.529 | 27.342 | 17.872 | 1.00 | 69.83 | 6 |
| | ATOM | 226 | CD | LYS A | 240 | 27.805 | 27.037 | 17.108 | 1.00 | 71.49 | 6 |
| 35 | ATOM | 227 | CE | LYS A | 240 | 28.980 | 27.720 | 17.776 | 1.00 | 71.31 | 6 |
| | ATOM | 228 | NZ | LYS A | 240 | 30.238 | 27.438 | 17.034 | 1.00 | 72.23 | 7 |
| | ATOM | 229 | C | LYS A | 240 | 22.808 | 26.699 | 16.895 | 1.00 | 66.19 | 6 |
| | ATOM | 230 | O | LYS A | 240 | 22.550 | 27.298 | 15.851 | 1.00 | 65.20 | 8 |
| | ATOM | 231 | N | ASN A | 241 | 22.113 | 25.640 | 17.325 | 1.00 | 66.69 | 7 |
| 40 | ATOM | 232 | CA | ASN A | 241 | 20.976 | 25.078 | 16.599 | 1.00 | 67.53 | 6 |
| | ATOM | 233 | CB | ASN A | 241 | 21.122 | 23.562 | 16.550 | 1.00 | 67.98 | 6 |
| | ATOM | 234 | CG | ASN A | 241 | 22.304 | 23.121 | 15.693 | 1.00 | 70.19 | 6 |
| | ATOM | 235 | OD1 | ASN A | 241 | 22.404 | 23.506 | 14.503 | 1.00 | 71.37 | 8 |
| | ATOM | 236 | ND2 | ASN A | 241 | 23.176 | 22.310 | 16.271 | 1.00 | 71.48 | 7 |
| 45 | ATOM | 237 | C | ASN A | 241 | 19.570 | 25.421 | 17.152 | 1.00 | 66.62 | 6 |
| | ATOM | 238 | O | ASN A | 241 | 18.581 | 24.822 | 16.731 | 1.00 | 64.76 | 8 |
| | ATOM | 239 | N | LYS A | 242 | 19.475 | 26.380 | 18.069 | 1.00 | 66.86 | 7 |
| | ATOM | 240 | CA | LYS A | 242 | 18.191 | 26.786 | 18.642 | 1.00 | 67.46 | 6 |
| | ATOM | 241 | CB | LYS A | 242 | 18.164 | 26.396 | 20.119 | 1.00 | 67.93 | 6 |
| 50 | ATOM | 242 | CG | LYS A | 242 | 18.250 | 24.896 | 20.337 | 1.00 | 71.52 | 6 |
| | ATOM | 243 | CD | LYS A | 242 | 17.004 | 24.149 | 19.821 | 1.00 | 74.32 | 6 |
| | ATOM | 244 | CE | LYS A | 242 | 15.755 | 24.491 | 20.643 | 1.00 | 74.41 | 6 |
| | ATOM | 245 | NZ | LYS A | 242 | 15.927 | 24.161 | 22.109 | 1.00 | 74.44 | 7 |
| | ATOM | 246 | C | LYS A | 242 | 18.143 | 28.291 | 18.483 | 1.00 | 66.28 | 6 |
| 55 | ATOM | 247 | O | LYS A | 242 | 17.102 | 28.923 | 18.592 | 1.00 | 67.61 | 8 |
| | ATOM | 248 | N | ARG A | 243 | 19.334 | 28.813 | 18.204 | 1.00 | 64.19 | 7 |
| | ATOM | 249 | CA | ARG A | 243 | 19.617 | 30.219 | 17.975 | 1.00 | 62.43 | 6 |
| | ATOM | 250 | CB | ARG A | 243 | 21.070 | 30.274 | 17.463 | 1.00 | 60.12 | 6 |

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|----|------|-----|-----|-----------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 251 | CG | ARG A 243 | 21.665 | 31.636 | 17.305 | 1.00 | 40.00 | 6 |
| | ATOM | 252 | CD | ARG A 243 | 23.213 | 31.599 | 17.267 | 1.00 | 40.00 | 6 |
| | ATOM | 253 | NE | ARG A 243 | 23.826 | 31.217 | 15.996 | 1.00 | 40.00 | 7 |
| | ATOM | 254 | CZ | ARG A 243 | 25.113 | 31.439 | 15.714 | 1.00 | 40.00 | 6 |
| | ATOM | 255 | NH1 | ARG A 243 | 25.905 | 32.041 | 16.616 | 1.00 | 40.00 | 7 |
| 10 | ATOM | 256 | NH2 | ARG A 243 | 25.592 | 31.097 | 14.520 | 1.00 | 40.00 | 7 |
| | ATOM | 257 | C | ARG A 243 | 18.639 | 30.789 | 16.950 | 1.00 | 62.97 | 6 |
| | ATOM | 258 | O | ARG A 243 | 18.662 | 30.390 | 15.784 | 1.00 | 63.96 | 8 |
| | ATOM | 259 | N | LYS A 244 | 17.771 | 31.692 | 17.393 | 1.00 | 62.41 | 7 |
| | ATOM | 260 | CA | LYS A 244 | 16.790 | 32.309 | 16.498 | 1.00 | 61.57 | 6 |
| 15 | ATOM | 261 | CB | LYS A 244 | 15.368 | 31.974 | 16.962 | 1.00 | 63.68 | 6 |
| | ATOM | 262 | CG | LYS A 244 | 15.102 | 30.471 | 17.104 | 1.00 | 71.29 | 6 |
| | ATOM | 263 | CD | LYS A 244 | 13.641 | 30.167 | 17.468 | 1.00 | 73.83 | 6 |
| | ATOM | 264 | CE | LYS A 244 | 13.182 | 30.908 | 18.737 | 1.00 | 74.71 | 6 |
| | ATOM | 265 | NZ | LYS A 244 | 13.951 | 30.536 | 19.970 | 1.00 | 73.32 | 7 |
| 20 | ATOM | 266 | C | LYS A 244 | 17.009 | 33.806 | 16.501 | 1.00 | 59.30 | 6 |
| | ATOM | 267 | O | LYS A 244 | 16.562 | 34.514 | 17.399 | 1.00 | 56.34 | 8 |
| | ATOM | 268 | N | PHE A 245 | 17.705 | 34.264 | 15.468 | 1.00 | 57.06 | 7 |
| | ATOM | 269 | CA | PHE A 245 | 18.045 | 35.692 | 15.333 | 1.00 | 59.01 | 6 |
| | ATOM | 270 | CB | PHE A 245 | 18.825 | 35.947 | 14.049 | 1.00 | 59.62 | 6 |
| 25 | ATOM | 271 | CG | PHE A 245 | 19.908 | 34.979 | 13.834 | 1.00 | 66.60 | 6 |
| | ATOM | 272 | CD1 | PHE A 245 | 19.618 | 33.714 | 13.399 | 1.00 | 67.17 | 6 |
| | ATOM | 273 | CD2 | PHE A 245 | 21.198 | 35.309 | 14.139 | 1.00 | 69.25 | 6 |
| | ATOM | 274 | CE1 | PHE A 245 | 20.614 | 32.794 | 13.255 | 1.00 | 69.92 | 6 |
| | ATOM | 275 | CE2 | PHE A 245 | 22.189 | 34.385 | 13.994 | 1.00 | 70.50 | 6 |
| 30 | ATOM | 276 | CZ | PHE A 245 | 21.897 | 33.126 | 13.552 | 1.00 | 70.89 | 6 |
| | ATOM | 277 | C | PHE A 245 | 16.856 | 36.620 | 15.340 | 1.00 | 60.68 | 6 |
| | ATOM | 278 | O | PHE A 245 | 15.946 | 36.516 | 14.528 | 1.00 | 62.37 | 8 |
| | ATOM | 279 | N | LEU A 246 | 16.919 | 37.558 | 16.272 | 1.00 | 60.10 | 7 |
| | ATOM | 280 | CA | LEU A 246 | 15.884 | 38.554 | 16.437 | 1.00 | 59.44 | 6 |
| 35 | ATOM | 281 | CB | LEU A 246 | 16.227 | 39.510 | 17.585 | 1.00 | 57.43 | 6 |
| | ATOM | 282 | CG | LEU A 246 | 15.100 | 40.384 | 18.086 | 1.00 | 54.41 | 6 |
| | ATOM | 283 | CD1 | LEU A 246 | 14.010 | 39.474 | 18.640 | 1.00 | 52.43 | 6 |
| | ATOM | 284 | CD2 | LEU A 246 | 15.575 | 41.325 | 19.151 | 1.00 | 51.69 | 6 |
| | ATOM | 285 | C | LEU A 246 | 15.717 | 39.330 | 15.135 | 1.00 | 62.05 | 6 |
| 40 | ATOM | 286 | O | LEU A 246 | 16.706 | 39.609 | 14.430 | 1.00 | 59.85 | 8 |
| | ATOM | 287 | N | PRO A 247 | 14.473 | 39.668 | 14.784 | 1.00 | 63.33 | 7 |
| | ATOM | 288 | CD | PRO A 247 | 13.263 | 39.314 | 15.534 | 1.00 | 64.44 | 6 |
| | ATOM | 289 | CA | PRO A 247 | 14.198 | 40.421 | 13.558 | 1.00 | 63.56 | 6 |
| | ATOM | 290 | CB | PRO A 247 | 12.687 | 40.671 | 13.600 | 1.00 | 64.42 | 6 |
| 45 | ATOM | 291 | CG | PRO A 247 | 12.161 | 39.922 | 14.729 | 1.00 | 64.90 | 6 |
| | ATOM | 292 | C | PRO A 247 | 14.996 | 41.733 | 13.496 | 1.00 | 61.94 | 6 |
| | ATOM | 293 | O | PRO A 247 | 15.159 | 42.455 | 14.486 | 1.00 | 61.60 | 8 |
| | ATOM | 294 | N | GLU A 248 | 15.506 | 42.006 | 12.299 | 1.00 | 61.33 | 7 |
| | ATOM | 295 | CA | GLU A 248 | 16.280 | 43.197 | 11.976 | 1.00 | 63.50 | 6 |
| 50 | ATOM | 296 | CB | GLU A 248 | 16.481 | 43.273 | 10.437 | 1.00 | 66.94 | 6 |
| | ATOM | 297 | CG | GLU A 248 | 17.012 | 44.671 | 9.966 | 1.00 | 68.70 | 6 |
| | ATOM | 298 | CD | GLU A 248 | 16.981 | 44.939 | 8.471 | 1.00 | 40.00 | 6 |
| | ATOM | 299 | OE1 | GLU A 248 | 16.432 | 44.144 | 7.644 | 1.00 | 40.00 | 8 |
| | ATOM | 300 | OE2 | GLU A 248 | 17.509 | 46.015 | 8.086 | 1.00 | 40.00 | 8 |
| 55 | ATOM | 301 | C | GLU A 248 | 15.624 | 44.489 | 12.458 | 1.00 | 64.19 | 6 |
| | ATOM | 302 | O | GLU A 248 | 16.298 | 45.395 | 12.918 | 1.00 | 65.56 | 8 |
| | ATOM | 303 | N | ASP A 249 | 14.300 | 44.545 | 12.323 | 1.00 | 64.36 | 7 |
| | ATOM | 304 | CA | ASP A 249 | 13.493 | 45.703 | 12.673 | 1.00 | 63.33 | 6 |

| | | | | | | | | | | | | |
|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 305 | CB | ASP | A | 249 | 12.088 | 45.531 | 12.116 | 1.00 | 62.97 | 6 |
| | ATOM | 306 | CG | ASP | A | 249 | 11.277 | 44.527 | 12.870 | 1.00 | 64.63 | 6 |
| | ATOM | 307 | OD1 | ASP | A | 249 | 11.687 | 43.352 | 12.963 | 1.00 | 64.84 | 8 |
| | ATOM | 308 | OD2 | ASP | A | 249 | 10.183 | 44.880 | 13.395 | 1.00 | 66.52 | 8 |
| | ATOM | 309 | C | ASP | A | 249 | 13.371 | 46.062 | 14.130 | 1.00 | 64.31 | 6 |
| 10 | ATOM | 310 | O | ASP | A | 249 | 13.310 | 47.250 | 14.468 | 1.00 | 64.73 | 8 |
| | ATOM | 311 | N | ILE | A | 250 | 13.274 | 45.049 | 14.997 | 1.00 | 63.09 | 7 |
| | ATOM | 312 | CA | ILE | A | 250 | 13.133 | 45.318 | 16.418 | 1.00 | 64.39 | 6 |
| | ATOM | 313 | CB | ILE | A | 250 | 13.035 | 44.034 | 17.214 | 1.00 | 65.79 | 6 |
| | ATOM | 314 | CG2 | ILE | A | 250 | 12.001 | 44.104 | 18.336 | 1.00 | 64.78 | 6 |
| 15 | ATOM | 315 | CG1 | ILE | A | 250 | 12.611 | 42.860 | 16.341 | 1.00 | 65.28 | 6 |
| | ATOM | 316 | CD1 | ILE | A | 250 | 11.753 | 41.852 | 17.088 | 1.00 | 65.08 | 6 |
| | ATOM | 317 | C | ILE | A | 250 | 14.404 | 46.104 | 17.276 | 1.00 | 65.21 | 6 |
| | ATOM | 318 | O | ILE | A | 250 | 15.155 | 45.506 | 18.047 | 1.00 | 64.05 | 8 |
| | ATOM | 319 | N | GLY | A | 251 | 14.670 | 47.529 | 17.299 | 1.00 | 65.48 | 7 |
| 20 | ATOM | 320 | CA | GLY | A | 251 | 15.871 | 48.326 | 18.042 | 1.00 | 67.32 | 6 |
| | ATOM | 321 | C | GLY | A | 251 | 16.595 | 49.110 | 16.895 | 1.00 | 68.52 | 6 |
| | ATOM | 322 | O | GLY | A | 251 | 17.528 | 48.616 | 16.266 | 1.00 | 65.49 | 8 |
| | ATOM | 323 | N | GLN | A | 252 | 16.162 | 50.356 | 16.557 | 1.00 | 72.26 | 7 |
| | ATOM | 324 | CA | GLN | A | 252 | 16.541 | 50.930 | 15.207 | 1.00 | 74.10 | 6 |
| 25 | ATOM | 325 | CB | GLN | A | 252 | 15.316 | 50.844 | 14.295 | 1.00 | 75.82 | 6 |
| | ATOM | 326 | C | GLN | A | 252 | 16.995 | 52.403 | 15.084 | 1.00 | 77.17 | 6 |
| | ATOM | 327 | O | GLN | A | 252 | 17.572 | 52.955 | 15.986 | 1.00 | 76.50 | 8 |
| | ATOM | 328 | N | ALA | A | 253 | 16.374 | 53.372 | 13.908 | 1.00 | 80.78 | 7 |
| | ATOM | 329 | CA | ALA | A | 253 | 16.687 | 54.725 | 13.567 | 1.00 | 83.70 | 6 |
| 30 | ATOM | 330 | CE | ALA | A | 253 | 16.381 | 54.956 | 12.093 | 1.00 | 83.23 | 6 |
| | ATOM | 331 | C | ALA | A | 253 | 16.159 | 55.960 | 14.345 | 1.00 | 85.59 | 6 |
| | ATOM | 332 | O | ALA | A | 253 | 15.317 | 56.721 | 13.798 | 1.00 | 85.69 | 8 |
| | ATOM | 333 | N | PRO | A | 254 | 16.384 | 56.155 | 16.264 | 1.00 | 35.05 | 7 |
| | ATOM | 334 | CD | PRO | A | 254 | 17.102 | 55.053 | 16.908 | 1.00 | 33.97 | 6 |
| 35 | ATOM | 335 | CA | PRO | A | 254 | 16.002 | 57.231 | 17.219 | 1.00 | 35.89 | 6 |
| | ATOM | 336 | CB | PRO | A | 254 | 16.534 | 56.756 | 18.563 | 1.00 | 33.94 | 6 |
| | ATOM | 337 | CG | PRO | A | 254 | 17.146 | 55.441 | 18.349 | 1.00 | 33.31 | 6 |
| | ATOM | 338 | C | PRO | A | 254 | 16.717 | 58.498 | 16.731 | 1.00 | 37.75 | 6 |
| | ATOM | 339 | O | PRO | A | 254 | 17.838 | 58.804 | 17.100 | 1.00 | 38.78 | 8 |
| 40 | TER | | | | | | | | | | | |
| | ATOM | 1 | N | LYS | A | 263 | 18.045 | 57.462 | 23.875 | 1.00 | 61.71 | 7 |
| | ATOM | 2 | CA | LYS | A | 263 | 16.824 | 56.712 | 24.215 | 1.00 | 64.36 | 6 |
| | ATOM | 3 | CB | LYS | A | 263 | 15.758 | 57.004 | 23.141 | 1.00 | 63.50 | 6 |
| | ATOM | 4 | C | LYS | A | 263 | 16.841 | 55.180 | 24.429 | 1.00 | 63.41 | 6 |
| 45 | ATOM | 5 | O | LYS | A | 263 | 17.877 | 54.542 | 24.409 | 1.00 | 61.93 | 8 |
| | ATOM | 6 | N | VAL | A | 264 | 15.615 | 54.664 | 24.654 | 1.00 | 61.15 | 7 |
| | ATOM | 7 | CA | VAL | A | 264 | 15.292 | 53.229 | 24.856 | 1.00 | 59.46 | 6 |
| | ATOM | 8 | CB | VAL | A | 264 | 14.251 | 52.974 | 25.978 | 1.00 | 59.03 | 6 |
| | ATOM | 9 | CG1 | VAL | A | 264 | 14.229 | 51.494 | 26.368 | 1.00 | 53.79 | 6 |
| 50 | ATOM | 10 | CG2 | VAL | A | 264 | 14.449 | 53.818 | 27.142 | 1.00 | 55.32 | 6 |
| | ATOM | 11 | C | VAL | A | 264 | 14.590 | 52.820 | 23.554 | 1.00 | 60.96 | 6 |
| | ATOM | 12 | O | VAL | A | 264 | 14.734 | 53.468 | 22.508 | 1.00 | 62.13 | 8 |
| | ATOM | 13 | N | ASP | A | 265 | 13.802 | 51.755 | 23.634 | 1.00 | 62.59 | 7 |
| | ATOM | 14 | CA | ASP | A | 265 | 12.995 | 51.263 | 22.526 | 1.00 | 64.95 | 6 |
| 55 | ATOM | 15 | CB | ASP | A | 265 | 13.825 | 51.077 | 21.271 | 1.00 | 64.32 | 6 |
| | ATOM | 16 | CG | ASP | A | 265 | 13.282 | 50.048 | 20.485 | 1.00 | 67.70 | 6 |
| | ATOM | 17 | OD1 | ASP | A | 265 | 12.795 | 50.011 | 19.446 | 1.00 | 72.59 | 8 |
| | ATOM | 18 | OD2 | ASP | A | 265 | 13.354 | 48.867 | 20.294 | 1.00 | 68.84 | 8 |

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|----|------|----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 19 | C | ASP | A | 265 | 12.326 | 49.943 | 22.952 | 1.00 | 65.64 | 6 |
| | ATOM | 20 | O | ASP | A | 265 | 12.771 | 48.850 | 22.655 | 1.00 | 68.81 | 8 |
| | ATOM | 21 | N | LEU | A | 266 | 11.256 | 50.152 | 23.702 | 1.00 | 65.12 | 7 |
| | ATOM | 22 | CA | LEU | A | 266 | 10.368 | 49.169 | 24.288 | 1.00 | 63.40 | 6 |
| | ATOM | 23 | CB | LEU | A | 266 | 9.115 | 49.938 | 24.708 | 1.00 | 67.34 | 6 |
| 10 | ATOM | 24 | CG | LEU | A | 266 | 9.399 | 51.124 | 25.618 | 1.00 | 69.35 | 6 |
| | ATOM | 25 | CD1 | LEU | A | 266 | 8.304 | 52.148 | 25.533 | 1.00 | 68.24 | 6 |
| | ATOM | 26 | CD2 | LEU | A | 266 | 9.581 | 50.631 | 27.021 | 1.00 | 70.47 | 6 |
| | ATOM | 27 | C | LEU | A | 266 | 9.940 | 47.888 | 23.559 | 1.00 | 59.67 | 6 |
| | ATOM | 28 | O | LEU | A | 266 | 9.694 | 46.879 | 24.220 | 1.00 | 53.35 | 8 |
| 15 | ATOM | 29 | N | GLU | A | 267 | 9.815 | 47.904 | 22.235 | 1.00 | 58.01 | 7 |
| | ATOM | 30 | CA | GLU | A | 267 | 9.417 | 46.682 | 21.572 | 1.00 | 58.34 | 6 |
| | ATOM | 31 | CB | GLU | A | 267 | 9.311 | 46.855 | 20.048 | 1.00 | 59.21 | 6 |
| | ATOM | 32 | CG | GLU | A | 267 | 9.129 | 45.494 | 19.322 | 1.00 | 62.89 | 6 |
| | ATOM | 33 | CD | GLU | A | 267 | 8.736 | 45.592 | 17.883 | 1.00 | 67.66 | 6 |
| 20 | ATOM | 34 | OE1 | GLU | A | 267 | 9.433 | 46.263 | 17.080 | 1.00 | 69.95 | 8 |
| | ATOM | 35 | OE2 | GLU | A | 267 | 7.710 | 44.974 | 17.503 | 1.00 | 69.40 | 8 |
| | ATOM | 36 | C | GLU | A | 267 | 10.504 | 45.683 | 21.895 | 1.00 | 57.67 | 6 |
| | ATOM | 37 | O | GLU | A | 267 | 10.255 | 44.485 | 21.988 | 1.00 | 58.34 | 8 |
| | ATOM | 38 | N | ALA | A | 268 | 11.712 | 46.222 | 22.054 | 1.00 | 53.43 | 7 |
| 25 | ATOM | 39 | CA | ALA | A | 268 | 12.903 | 45.454 | 22.374 | 1.00 | 49.00 | 6 |
| | ATOM | 40 | CB | ALA | A | 268 | 14.137 | 46.241 | 21.983 | 1.00 | 45.72 | 6 |
| | ATOM | 41 | C | ALA | A | 268 | 12.908 | 45.196 | 23.873 | 1.00 | 45.76 | 6 |
| | ATOM | 42 | O | ALA | A | 268 | 12.887 | 44.042 | 24.307 | 1.00 | 41.50 | 8 |
| | ATOM | 43 | N | PHE | A | 269 | 12.918 | 46.277 | 24.663 | 1.00 | 41.43 | 7 |
| 30 | ATOM | 44 | CA | PHE | A | 269 | 12.920 | 46.158 | 26.118 | 1.00 | 43.96 | 6 |
| | ATOM | 45 | CB | PHE | A | 269 | 12.395 | 47.426 | 26.777 | 1.00 | 40.10 | 6 |
| | ATOM | 46 | CG | PHE | A | 269 | 12.332 | 47.345 | 28.271 | 1.00 | 40.44 | 6 |
| | ATOM | 47 | CD1 | PHE | A | 269 | 13.457 | 47.595 | 29.034 | 1.00 | 38.98 | 6 |
| | ATOM | 48 | CD2 | PHE | A | 269 | 11.165 | 46.946 | 28.903 | 1.00 | 37.15 | 6 |
| 35 | ATOM | 49 | CE1 | PHE | A | 269 | 13.409 | 47.469 | 30.436 | 1.00 | 32.12 | 6 |
| | ATOM | 50 | CE2 | PHE | A | 269 | 11.105 | 46.815 | 30.303 | 1.00 | 38.41 | 6 |
| | ATOM | 51 | CZ | PHE | A | 269 | 12.228 | 47.070 | 31.071 | 1.00 | 40.55 | 6 |
| | ATOM | 52 | C | PHE | A | 269 | 12.017 | 45.012 | 26.520 | 1.00 | 49.76 | 6 |
| | ATOM | 53 | O | PHE | A | 269 | 12.277 | 44.324 | 27.484 | 1.00 | 52.15 | 8 |
| 40 | ATOM | 54 | N | SER | A | 270 | 10.934 | 44.835 | 25.768 | 1.00 | 53.15 | 7 |
| | ATOM | 55 | CA | SER | A | 270 | 9.988 | 43.768 | 26.043 | 1.00 | 52.29 | 6 |
| | ATOM | 56 | CB | SER | A | 270 | 8.727 | 43.943 | 25.215 | 1.00 | 51.85 | 6 |
| | ATOM | 57 | OG | SER | A | 270 | 7.785 | 42.918 | 25.497 | 1.00 | 53.42 | 8 |
| | ATOM | 58 | C | SER | A | 270 | 10.637 | 42.464 | 25.685 | 1.00 | 49.38 | 6 |
| 45 | ATOM | 59 | O | SER | A | 270 | 11.068 | 41.741 | 26.562 | 1.00 | 48.74 | 8 |
| | ATOM | 60 | N | HIS | A | 271 | 10.683 | 42.173 | 24.383 | 1.00 | 50.15 | 7 |
| | ATOM | 61 | CA | HIS | A | 271 | 11.276 | 40.932 | 23.877 | 1.00 | 51.67 | 6 |
| | ATOM | 62 | CB | HIS | A | 271 | 11.797 | 41.118 | 22.455 | 1.00 | 58.52 | 6 |
| | ATOM | 63 | CG | HIS | A | 271 | 10.775 | 40.885 | 21.399 | 1.00 | 68.97 | 6 |
| 50 | ATOM | 64 | CD2 | HIS | A | 271 | 10.633 | 39.891 | 20.485 | 1.00 | 70.88 | 6 |
| | ATOM | 65 | ND1 | HIS | A | 271 | 9.673 | 41.732 | 21.199 | 1.00 | 71.98 | 7 |
| | ATOM | 66 | CE1 | HIS | A | 271 | 8.936 | 41.242 | 20.209 | 1.00 | 73.91 | 6 |
| | ATOM | 67 | NE2 | HIS | A | 271 | 9.495 | 40.132 | 19.764 | 1.00 | 73.59 | 7 |
| | ATOM | 68 | C | HIS | A | 271 | 12.402 | 40.416 | 24.745 | 1.00 | 48.33 | 6 |
| 55 | ATOM | 69 | O | HIS | A | 271 | 12.707 | 39.225 | 24.728 | 1.00 | 48.39 | 8 |
| | ATOM | 70 | N | PHE | A | 272 | 13.029 | 41.334 | 25.487 | 1.00 | 41.34 | 7 |
| | ATOM | 71 | CA | PHE | A | 272 | 14.130 | 41.001 | 26.384 | 1.00 | 39.44 | 6 |
| | ATOM | 72 | CB | PHE | A | 272 | 15.077 | 42.194 | 26.512 | 1.00 | 36.67 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 73 | CG | PHE | A | 272 | 15.953 | 42.413 | 25.282 | 1.00 | 33.39 | 6 |
| | ATOM | 74 | CD1 | PHE | A | 272 | 16.619 | 43.615 | 25.093 | 1.00 | 33.14 | 6 |
| | ATOM | 75 | CD2 | PHE | A | 272 | 16.138 | 41.394 | 24.346 | 1.00 | 38.28 | 6 |
| | ATOM | 76 | CE1 | PHE | A | 272 | 17.454 | 43.807 | 23.988 | 1.00 | 38.26 | 6 |
| | ATOM | 77 | CE2 | PHE | A | 272 | 16.973 | 41.585 | 23.244 | 1.00 | 43.28 | 6 |
| 10 | ATOM | 78 | CZ | PHE | A | 272 | 17.634 | 42.786 | 23.068 | 1.00 | 39.74 | 6 |
| | ATOM | 79 | C | PHE | A | 272 | 13.650 | 40.528 | 27.764 | 1.00 | 40.75 | 6 |
| | ATOM | 80 | O | PHE | A | 272 | 14.081 | 39.476 | 28.227 | 1.00 | 35.51 | 8 |
| | ATOM | 81 | N | THR | A | 273 | 12.756 | 41.266 | 28.428 | 1.00 | 41.64 | 7 |
| | ATOM | 82 | CA | THR | A | 273 | 12.290 | 40.854 | 29.757 | 1.00 | 45.97 | 6 |
| 15 | ATOM | 83 | CB | THR | A | 273 | 11.651 | 42.025 | 30.506 | 1.00 | 51.52 | 6 |
| | ATOM | 84 | OG1 | THR | A | 273 | 10.442 | 42.422 | 29.859 | 1.00 | 45.74 | 8 |
| | ATOM | 85 | CG2 | THR | A | 273 | 12.601 | 43.211 | 30.565 | 1.00 | 49.73 | 6 |
| | ATOM | 86 | C | THR | A | 273 | 11.267 | 39.731 | 29.664 | 1.00 | 46.23 | 6 |
| | ATOM | 87 | O | THR | A | 273 | 10.854 | 39.183 | 30.680 | 1.00 | 41.21 | 8 |
| 20 | ATOM | 88 | N | LYS | A | 274 | 10.849 | 39.412 | 28.440 | 1.00 | 46.21 | 7 |
| | ATOM | 89 | CA | LYS | A | 274 | 9.871 | 38.362 | 28.211 | 1.00 | 54.53 | 6 |
| | ATOM | 90 | CB | LYS | A | 274 | 9.414 | 38.405 | 26.773 | 1.00 | 54.36 | 6 |
| | ATOM | 91 | C | LYS | A | 274 | 10.498 | 37.015 | 28.515 | 1.00 | 56.88 | 6 |
| | ATOM | 92 | O | LYS | A | 274 | 9.789 | 36.044 | 28.759 | 1.00 | 57.98 | 8 |
| 25 | ATOM | 93 | N | ILE | A | 275 | 11.836 | 36.973 | 28.491 | 1.00 | 56.48 | 7 |
| | ATOM | 94 | CA | ILE | A | 275 | 12.609 | 35.746 | 28.767 | 1.00 | 52.64 | 6 |
| | ATOM | 95 | CB | ILE | A | 275 | 13.444 | 35.346 | 27.543 | 1.00 | 49.15 | 6 |
| | ATOM | 96 | CG2 | ILE | A | 275 | 12.568 | 34.829 | 26.429 | 1.00 | 47.42 | 6 |
| | ATOM | 97 | CG1 | ILE | A | 275 | 14.238 | 36.532 | 27.026 | 1.00 | 45.31 | 6 |
| 30 | ATOM | 98 | CD1 | ILE | A | 275 | 15.001 | 36.242 | 25.771 | 1.00 | 37.22 | 6 |
| | ATOM | 99 | C | ILE | A | 275 | 13.541 | 35.870 | 29.982 | 1.00 | 51.78 | 6 |
| | ATOM | 100 | O | ILE | A | 275 | 14.014 | 34.873 | 30.503 | 1.00 | 49.80 | 8 |
| | ATOM | 101 | N | ILE | A | 276 | 13.790 | 37.107 | 30.415 | 1.00 | 51.76 | 7 |
| | ATOM | 102 | CA | ILE | A | 276 | 14.681 | 37.389 | 31.537 | 1.00 | 52.58 | 6 |
| 35 | ATOM | 103 | CB | ILE | A | 276 | 14.691 | 38.877 | 31.844 | 1.00 | 55.04 | 6 |
| | ATOM | 104 | CG2 | ILE | A | 276 | 13.311 | 39.340 | 32.261 | 1.00 | 53.28 | 6 |
| | ATOM | 105 | CG1 | ILE | A | 276 | 15.675 | 39.206 | 32.976 | 1.00 | 57.31 | 6 |
| | ATOM | 106 | CD1 | ILE | A | 276 | 17.096 | 38.942 | 32.655 | 1.00 | 60.32 | 6 |
| | ATOM | 107 | C | ILE | A | 276 | 14.323 | 36.644 | 32.828 | 1.00 | 50.70 | 6 |
| 40 | ATOM | 108 | O | ILE | A | 276 | 15.177 | 36.458 | 33.691 | 1.00 | 55.55 | 8 |
| | ATOM | 109 | N | THR | A | 277 | 13.072 | 36.209 | 32.963 | 1.00 | 47.33 | 7 |
| | ATOM | 110 | CA | THR | A | 277 | 12.631 | 35.523 | 34.158 | 1.00 | 42.59 | 6 |
| | ATOM | 111 | CB | THR | A | 277 | 11.098 | 35.456 | 34.217 | 1.00 | 44.97 | 6 |
| | ATOM | 112 | OG1 | THR | A | 277 | 10.545 | 36.777 | 34.102 | 1.00 | 46.38 | 8 |
| 45 | ATOM | 113 | CG2 | THR | A | 277 | 10.657 | 34.838 | 35.539 | 1.00 | 37.17 | 6 |
| | ATOM | 114 | C | THR | A | 277 | 13.211 | 34.118 | 34.304 | 1.00 | 39.84 | 6 |
| | ATOM | 115 | O | THR | A | 277 | 13.796 | 33.796 | 35.365 | 1.00 | 40.55 | 8 |
| | ATOM | 116 | N | PRO | A | 278 | 13.055 | 33.261 | 33.288 | 1.00 | 38.20 | 7 |
| | ATOM | 117 | CD | PRO | A | 278 | 12.370 | 33.534 | 32.023 | 1.00 | 36.34 | 6 |
| 50 | ATOM | 118 | CA | PRO | A | 278 | 13.595 | 31.894 | 33.363 | 1.00 | 36.63 | 6 |
| | ATOM | 119 | CB | PRO | A | 278 | 13.153 | 31.244 | 32.064 | 1.00 | 32.95 | 6 |
| | ATOM | 120 | CG | PRO | A | 278 | 12.573 | 32.291 | 31.239 | 1.00 | 35.75 | 6 |
| | ATOM | 121 | C | PRO | A | 278 | 15.101 | 31.932 | 33.476 | 1.00 | 38.60 | 6 |
| | ATOM | 122 | O | PRO | A | 278 | 15.746 | 30.981 | 33.898 | 1.00 | 37.67 | 8 |
| 55 | ATOM | 123 | N | ALA | A | 279 | 15.656 | 33.051 | 33.035 | 1.00 | 37.05 | 7 |
| | ATOM | 124 | CA | ALA | A | 279 | 17.087 | 33.277 | 33.041 | 1.00 | 33.18 | 6 |
| | ATOM | 125 | CB | ALA | A | 279 | 17.376 | 34.599 | 32.348 | 1.00 | 30.56 | 6 |
| | ATOM | 126 | C | ALA | A | 279 | 17.624 | 33.312 | 34.452 | 1.00 | 33.47 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 127 | O | ALA | A | 279 | 18.523 | 32.555 | 34.789 | 1.00 | 33.74 | 8 |
| | ATOM | 128 | N | ILE | A | 280 | 17.060 | 34.215 | 35.260 | 1.00 | 29.96 | 7 |
| | ATOM | 129 | CA | ILE | A | 280 | 17.459 | 34.362 | 36.646 | 1.00 | 25.94 | 6 |
| | ATOM | 130 | CB | ILE | A | 280 | 16.686 | 35.484 | 37.315 | 1.00 | 26.95 | 6 |
| | ATOM | 131 | CG2 | ILE | A | 280 | 17.109 | 35.632 | 38.733 | 1.00 | 15.40 | 6 |
| 10 | ATOM | 132 | CG1 | ILE | A | 280 | 16.931 | 36.808 | 36.595 | 1.00 | 26.73 | 6 |
| | ATOM | 133 | CD1 | ILE | A | 280 | 16.292 | 38.002 | 37.272 | 1.00 | 34.31 | 6 |
| | ATOM | 134 | C | ILE | A | 280 | 17.263 | 33.066 | 37.412 | 1.00 | 31.39 | 6 |
| | ATOM | 135 | O | ILE | A | 280 | 18.116 | 32.679 | 38.207 | 1.00 | 35.69 | 8 |
| | ATOM | 136 | N | THR | A | 281 | 16.145 | 32.386 | 37.165 | 1.00 | 30.90 | 7 |
| 15 | ATOM | 137 | CA | THR | A | 281 | 15.854 | 31.118 | 37.851 | 1.00 | 33.49 | 6 |
| | ATOM | 138 | CB | THR | A | 281 | 14.598 | 30.413 | 37.277 | 1.00 | 37.18 | 6 |
| | ATOM | 139 | OG1 | THR | A | 281 | 14.795 | 30.099 | 35.898 | 1.00 | 46.48 | 8 |
| | ATOM | 140 | CG2 | THR | A | 281 | 13.352 | 31.281 | 37.444 | 1.00 | 32.85 | 6 |
| | ATOM | 141 | C | THR | A | 281 | 17.045 | 30.176 | 37.713 | 1.00 | 29.94 | 6 |
| 20 | ATOM | 142 | O | THR | A | 281 | 17.478 | 29.546 | 38.684 | 1.00 | 25.55 | 8 |
| | ATOM | 143 | N | ARG | A | 282 | 17.561 | 30.076 | 36.489 | 1.00 | 32.70 | 7 |
| | ATOM | 144 | CA | ARG | A | 282 | 18.692 | 29.198 | 36.218 | 1.00 | 34.27 | 6 |
| | ATOM | 145 | CB | ARG | A | 282 | 19.136 | 29.374 | 34.780 | 1.00 | 33.78 | 6 |
| | ATOM | 146 | CG | ARG | A | 282 | 19.272 | 28.086 | 34.013 | 1.00 | 45.15 | 6 |
| 25 | ATOM | 147 | CD | ARG | A | 282 | 18.179 | 27.921 | 32.977 | 1.00 | 58.24 | 6 |
| | ATOM | 148 | NE | ARG | A | 282 | 18.041 | 29.077 | 32.117 | 1.00 | 68.41 | 7 |
| | ATOM | 149 | CZ | ARG | A | 282 | 19.018 | 29.529 | 31.352 | 1.00 | 72.31 | 6 |
| | ATOM | 150 | NH1 | ARG | A | 282 | 20.190 | 28.886 | 31.327 | 1.00 | 77.89 | 7 |
| | ATOM | 151 | NH2 | ARG | A | 282 | 18.802 | 30.593 | 30.595 | 1.00 | 69.25 | 7 |
| 30 | ATOM | 152 | C | ARG | A | 282 | 19.823 | 29.582 | 37.170 | 1.00 | 34.81 | 6 |
| | ATOM | 153 | O | ARG | A | 282 | 20.380 | 28.735 | 37.855 | 1.00 | 36.03 | 8 |
| | ATOM | 154 | N | VAL | A | 283 | 20.135 | 30.882 | 37.190 | 1.00 | 31.71 | 7 |
| | ATOM | 155 | CA | VAL | A | 283 | 21.171 | 31.434 | 38.057 | 1.00 | 30.16 | 6 |
| | ATOM | 156 | CB | VAL | A | 283 | 21.198 | 32.965 | 37.981 | 1.00 | 29.00 | 6 |
| 35 | ATOM | 157 | CG1 | VAL | A | 283 | 22.208 | 33.533 | 38.952 | 1.00 | 28.64 | 6 |
| | ATOM | 158 | CG2 | VAL | A | 283 | 21.525 | 33.415 | 36.578 | 1.00 | 28.28 | 6 |
| | ATOM | 159 | C | VAL | A | 283 | 20.942 | 30.992 | 39.498 | 1.00 | 32.50 | 6 |
| | ATOM | 160 | O | VAL | A | 283 | 21.879 | 30.717 | 40.229 | 1.00 | 33.48 | 8 |
| | ATOM | 161 | N | VAL | A | 284 | 19.671 | 30.941 | 39.892 | 1.00 | 30.96 | 7 |
| 40 | ATOM | 162 | CA | VAL | A | 284 | 19.289 | 30.527 | 41.239 | 1.00 | 29.14 | 6 |
| | ATOM | 163 | CB | VAL | A | 284 | 17.822 | 30.865 | 41.548 | 1.00 | 31.27 | 6 |
| | ATOM | 164 | CG1 | VAL | A | 284 | 17.472 | 30.461 | 42.945 | 1.00 | 24.21 | 6 |
| | ATOM | 165 | CG2 | VAL | A | 284 | 17.555 | 32.334 | 41.360 | 1.00 | 30.51 | 6 |
| | ATOM | 166 | C | VAL | A | 284 | 19.529 | 29.037 | 41.353 | 1.00 | 28.89 | 6 |
| 45 | ATOM | 167 | O | VAL | A | 284 | 20.073 | 28.568 | 42.345 | 1.00 | 27.29 | 8 |
| | ATOM | 168 | N | ASP | A | 285 | 19.121 | 28.296 | 40.327 | 1.00 | 28.76 | 7 |
| | ATOM | 169 | CA | ASP | A | 285 | 19.277 | 26.842 | 40.306 | 1.00 | 35.32 | 6 |
| | ATOM | 170 | CB | ASP | A | 285 | 18.586 | 26.234 | 39.072 | 1.00 | 33.29 | 6 |
| | ATOM | 171 | CG | ASP | A | 285 | 17.083 | 26.277 | 39.149 | 1.00 | 38.15 | 6 |
| 50 | ATOM | 172 | OD1 | ASP | A | 285 | 16.484 | 25.743 | 40.110 | 1.00 | 34.70 | 8 |
| | ATOM | 173 | OD2 | ASP | A | 285 | 16.431 | 26.828 | 38.231 | 1.00 | 34.43 | 8 |
| | ATOM | 174 | C | ASP | A | 285 | 20.751 | 26.449 | 40.305 | 1.00 | 36.70 | 6 |
| | ATOM | 175 | O | ASP | A | 285 | 21.106 | 25.389 | 40.808 | 1.00 | 37.96 | 8 |
| | ATOM | 176 | N | PHE | A | 286 | 21.604 | 27.300 | 39.737 | 1.00 | 35.96 | 7 |
| 55 | ATOM | 177 | CA | PHE | A | 286 | 23.029 | 27.022 | 39.704 | 1.00 | 37.10 | 6 |
| | ATOM | 178 | CB | PHE | A | 286 | 23.754 | 28.009 | 38.793 | 1.00 | 37.97 | 6 |
| | ATOM | 179 | CG | PHE | A | 286 | 25.252 | 28.027 | 38.987 | 1.00 | 36.50 | 6 |
| | ATOM | 180 | CD1 | PHE | A | 286 | 25.963 | 26.849 | 38.974 | 1.00 | 36.75 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| 5 | ATOM | 181 | CD2 | PHE | A | 286 | 25.931 | 29.218 | 39.199 | 1.00 | 33.83 | 6 |
| | ATOM | 182 | CE1 | PHE | A | 286 | 27.331 | 26.860 | 39.161 | 1.00 | 39.55 | 6 |
| | ATOM | 183 | CE2 | PHE | A | 286 | 27.307 | 29.233 | 39.387 | 1.00 | 38.08 | 6 |
| | ATOM | 184 | CZ | PHE | A | 286 | 28.008 | 28.052 | 39.371 | 1.00 | 34.44 | 6 |
| | ATOM | 185 | C | PHE | A | 286 | 23.631 | 27.105 | 41.083 | 1.00 | 36.83 | 6 |
| 10 | ATOM | 186 | O | PHE | A | 286 | 24.317 | 26.192 | 41.504 | 1.00 | 35.61 | 8 |
| | ATOM | 187 | N | ALA | A | 287 | 23.393 | 28.228 | 41.752 | 1.00 | 37.33 | 7 |
| | ATOM | 188 | CA | ALA | A | 287 | 23.917 | 28.448 | 43.087 | 1.00 | 36.34 | 6 |
| | ATOM | 189 | CB | ALA | A | 287 | 23.523 | 29.828 | 43.555 | 1.00 | 36.40 | 6 |
| | ATOM | 190 | C | ALA | A | 287 | 23.346 | 27.393 | 44.027 | 1.00 | 38.76 | 6 |
| 15 | ATOM | 191 | O | ALA | A | 287 | 23.994 | 26.973 | 44.981 | 1.00 | 41.98 | 8 |
| | ATOM | 192 | N | LYS | A | 288 | 22.114 | 26.979 | 43.735 | 1.00 | 38.28 | 7 |
| | ATOM | 193 | CA | LYS | A | 288 | 21.429 | 25.971 | 44.538 | 1.00 | 45.26 | 6 |
| | ATOM | 194 | CB | LYS | A | 288 | 19.994 | 25.746 | 44.054 | 1.00 | 48.35 | 6 |
| | ATOM | 195 | CG | LYS | A | 288 | 19.025 | 26.819 | 44.464 | 1.00 | 51.43 | 6 |
| 20 | ATOM | 196 | CD | LYS | A | 288 | 17.628 | 26.246 | 44.682 | 1.00 | 60.23 | 6 |
| | ATOM | 197 | CE | LYS | A | 288 | 17.135 | 25.478 | 43.485 | 1.00 | 62.81 | 6 |
| | ATOM | 198 | NZ | LYS | A | 288 | 17.196 | 26.327 | 42.268 | 1.00 | 64.69 | 7 |
| | ATOM | 199 | C | LYS | A | 288 | 22.120 | 24.632 | 44.536 | 1.00 | 43.31 | 6 |
| | ATOM | 200 | O | LYS | A | 288 | 21.967 | 23.857 | 45.462 | 1.00 | 45.66 | 8 |
| 25 | ATOM | 201 | N | LYS | A | 289 | 22.865 | 24.366 | 43.467 | 1.00 | 41.70 | 7 |
| | ATOM | 202 | CA | LYS | A | 289 | 23.571 | 23.120 | 43.351 | 1.00 | 40.67 | 6 |
| | ATOM | 203 | CB | LYS | A | 289 | 23.655 | 22.708 | 41.877 | 1.00 | 42.25 | 6 |
| | ATOM | 204 | CG | LYS | A | 289 | 22.271 | 22.492 | 41.247 | 1.00 | 39.53 | 6 |
| | ATOM | 205 | CD | LYS | A | 289 | 22.331 | 21.606 | 40.012 | 1.00 | 43.19 | 6 |
| 30 | ATOM | 206 | CE | LYS | A | 289 | 20.941 | 21.362 | 39.447 | 1.00 | 45.74 | 6 |
| | ATOM | 207 | NZ | LYS | A | 289 | 20.273 | 20.165 | 40.006 | 1.00 | 52.49 | 7 |
| | ATOM | 208 | C | LYS | A | 289 | 24.948 | 23.185 | 44.003 | 1.00 | 41.50 | 6 |
| | ATOM | 209 | O | LYS | A | 289 | 25.642 | 22.184 | 44.080 | 1.00 | 39.77 | 8 |
| | ATOM | 210 | N | LEU | A | 290 | 25.312 | 24.370 | 44.490 | 1.00 | 40.68 | 7 |
| 35 | ATOM | 211 | CA | LEU | A | 290 | 26.594 | 24.583 | 45.149 | 1.00 | 39.33 | 6 |
| | ATOM | 212 | CB | LEU | A | 290 | 27.153 | 25.972 | 44.829 | 1.00 | 36.14 | 6 |
| | ATOM | 213 | CG | LEU | A | 290 | 27.358 | 26.290 | 43.365 | 1.00 | 34.81 | 6 |
| | ATOM | 214 | CD1 | LEU | A | 290 | 27.945 | 27.675 | 43.208 | 1.00 | 29.07 | 6 |
| | ATOM | 215 | CD2 | LEU | A | 290 | 28.267 | 25.242 | 42.757 | 1.00 | 33.45 | 6 |
| 40 | ATOM | 216 | C | LEU | A | 290 | 26.434 | 24.405 | 46.652 | 1.00 | 40.08 | 6 |
| | ATOM | 217 | O | LEU | A | 290 | 25.803 | 25.235 | 47.333 | 1.00 | 42.00 | 8 |
| | ATOM | 218 | N | PRO | A | 291 | 27.028 | 23.333 | 47.210 | 1.00 | 40.27 | 7 |
| | ATOM | 219 | CD | PRO | A | 291 | 27.851 | 22.330 | 46.519 | 1.00 | 39.65 | 6 |
| | ATOM | 220 | CA | PRO | A | 291 | 26.905 | 23.096 | 48.659 | 1.00 | 38.28 | 6 |
| 45 | ATOM | 221 | CB | PRO | A | 291 | 27.755 | 21.860 | 48.911 | 1.00 | 35.88 | 6 |
| | ATOM | 222 | CG | PRO | A | 291 | 28.202 | 21.355 | 47.585 | 1.00 | 34.19 | 6 |
| | ATOM | 223 | C | PRO | A | 291 | 27.327 | 24.298 | 49.522 | 1.00 | 40.05 | 6 |
| | ATOM | 224 | O | PRO | A | 291 | 26.571 | 24.739 | 50.391 | 1.00 | 41.33 | 8 |
| | ATOM | 225 | N | MET | A | 292 | 28.522 | 24.843 | 49.299 | 1.00 | 40.59 | 7 |
| 50 | ATOM | 226 | CA | MET | A | 292 | 29.021 | 25.957 | 50.097 | 1.00 | 42.86 | 6 |
| | ATOM | 227 | CB | MET | A | 292 | 30.313 | 26.475 | 49.477 | 1.00 | 43.28 | 6 |
| | ATOM | 228 | CG | MET | A | 292 | 31.269 | 25.378 | 49.050 | 1.00 | 50.35 | 6 |
| | ATOM | 229 | SD | MET | A | 292 | 32.895 | 26.096 | 48.757 | 1.00 | 51.17 | 16 |
| | ATOM | 230 | CE | MET | A | 292 | 33.812 | 24.647 | 48.074 | 1.00 | 54.63 | 6 |
| 55 | ATOM | 231 | C | MET | A | 292 | 27.984 | 27.066 | 50.149 | 1.00 | 41.05 | 6 |
| | ATOM | 232 | O | MET | A | 292 | 27.986 | 27.886 | 51.057 | 1.00 | 39.66 | 8 |
| | ATOM | 233 | N | PHE | A | 293 | 27.080 | 27.078 | 49.172 | 1.00 | 39.30 | 7 |
| | ATOM | 234 | CA | PHE | A | 293 | 26.030 | 28.091 | 49.114 | 1.00 | 40.92 | 6 |

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|----|------|-----|-----|-----------|--------|--------|--------|------|-------|----|
| 5 | ATOM | 235 | CB | PHE A 293 | 25.398 | 28.107 | 47.715 | 1.00 | 40.98 | 6 |
| | ATOM | 236 | CG | PHE A 293 | 24.348 | 29.168 | 47.524 | 1.00 | 42.78 | 6 |
| | ATOM | 237 | CD1 | PHE A 293 | 24.654 | 30.493 | 47.747 | 1.00 | 44.40 | 6 |
| | ATOM | 238 | CD2 | PHE A 293 | 23.071 | 28.833 | 47.116 | 1.00 | 43.66 | 6 |
| | ATOM | 239 | CE1 | PHE A 293 | 23.701 | 31.478 | 47.564 | 1.00 | 39.83 | 6 |
| 10 | ATOM | 240 | CE2 | PHE A 293 | 22.112 | 29.819 | 46.930 | 1.00 | 46.21 | 6 |
| | ATOM | 241 | CZ | PHE A 293 | 22.430 | 31.146 | 47.155 | 1.00 | 45.18 | 6 |
| | ATOM | 242 | C | PHE A 293 | 24.979 | 27.772 | 50.164 | 1.00 | 45.54 | 6 |
| | ATOM | 243 | O | PHE A 293 | 24.686 | 28.576 | 51.034 | 1.00 | 42.01 | 8 |
| | ATOM | 244 | N | CYS A 294 | 24.426 | 26.572 | 50.062 | 1.00 | 47.05 | 7 |
| 15 | ATOM | 245 | CA | CYS A 294 | 23.386 | 26.125 | 50.962 | 1.00 | 50.15 | 6 |
| | ATOM | 246 | CB | CYS A 294 | 22.944 | 24.733 | 50.524 | 1.00 | 45.90 | 6 |
| | ATOM | 247 | SG | CYS A 294 | 22.303 | 24.663 | 48.829 | 1.00 | 51.50 | 16 |
| | ATOM | 248 | C | CYS A 294 | 23.825 | 26.125 | 52.423 | 1.00 | 51.38 | 6 |
| | ATOM | 249 | O | CYS A 294 | 23.008 | 25.954 | 53.322 | 1.00 | 53.83 | 8 |
| 20 | ATOM | 250 | N | GLU A 295 | 25.119 | 26.327 | 52.645 | 1.00 | 49.72 | 7 |
| | ATOM | 251 | CA | GLU A 295 | 25.666 | 26.384 | 53.996 | 1.00 | 52.53 | 6 |
| | ATOM | 252 | CB | GLU A 295 | 27.103 | 25.830 | 54.015 | 1.00 | 57.40 | 6 |
| | ATOM | 253 | CG | GLU A 295 | 27.182 | 24.309 | 54.061 | 1.00 | 69.63 | 6 |
| | ATOM | 254 | CD | GLU A 295 | 26.660 | 23.747 | 55.342 | 1.00 | 78.49 | 6 |
| 25 | ATOM | 255 | OE1 | GLU A 295 | 27.291 | 23.946 | 56.412 | 1.00 | 82.82 | 8 |
| | ATOM | 256 | OE2 | GLU A 295 | 25.590 | 23.086 | 55.335 | 1.00 | 85.30 | 8 |
| | ATOM | 257 | C | GLU A 295 | 25.653 | 27.831 | 54.488 | 1.00 | 48.54 | 6 |
| | ATOM | 258 | O | GLU A 295 | 26.365 | 28.184 | 55.426 | 1.00 | 49.82 | 8 |
| | ATOM | 259 | N | LEU A 296 | 24.804 | 28.631 | 53.846 | 1.00 | 43.79 | 7 |
| 30 | ATOM | 260 | CA | LEU A 296 | 24.670 | 30.034 | 54.159 | 1.00 | 45.42 | 6 |
| | ATOM | 261 | CB | LEU A 296 | 25.062 | 30.864 | 52.923 | 1.00 | 41.04 | 6 |
| | ATOM | 262 | CG | LEU A 296 | 26.438 | 30.658 | 52.315 | 1.00 | 42.74 | 6 |
| | ATOM | 263 | CD1 | LEU A 296 | 26.447 | 31.030 | 50.861 | 1.00 | 40.99 | 6 |
| | ATOM | 264 | CD2 | LEU A 296 | 27.437 | 31.454 | 53.086 | 1.00 | 39.44 | 6 |
| 35 | ATOM | 265 | C | LEU A 296 | 23.239 | 30.366 | 54.548 | 1.00 | 45.56 | 6 |
| | ATOM | 266 | O | LEU A 296 | 22.301 | 29.660 | 54.148 | 1.00 | 43.07 | 8 |
| | ATOM | 267 | N | PRO A 297 | 23.050 | 31.405 | 55.365 | 1.00 | 46.99 | 7 |
| | ATOM | 268 | CD | PRO A 297 | 24.121 | 32.241 | 55.930 | 1.00 | 47.12 | 6 |
| | ATOM | 269 | CA | PRO A 297 | 21.700 | 31.811 | 55.787 | 1.00 | 49.61 | 6 |
| 40 | ATOM | 270 | CB | PRO A 297 | 21.937 | 32.990 | 56.738 | 1.00 | 49.91 | 6 |
| | ATOM | 271 | CG | PRO A 297 | 23.401 | 33.155 | 56.872 | 1.00 | 51.28 | 6 |
| | ATOM | 272 | C | PRO A 297 | 20.864 | 32.212 | 54.558 | 1.00 | 49.59 | 6 |
| | ATOM | 273 | O | PRO A 297 | 21.402 | 32.684 | 53.556 | 1.00 | 51.66 | 8 |
| | ATOM | 274 | N | CYS A 298 | 19.545 | 32.035 | 54.655 | 1.00 | 51.02 | 7 |
| 45 | ATOM | 275 | CA | CYS A 298 | 18.618 | 32.369 | 53.567 | 1.00 | 52.86 | 6 |
| | ATOM | 276 | CB | CYS A 298 | 17.201 | 31.877 | 53.915 | 1.00 | 54.57 | 6 |
| | ATOM | 277 | SG | CYS A 298 | 16.040 | 33.162 | 54.440 | 1.00 | 67.87 | 16 |
| | ATOM | 278 | C | CYS A 298 | 18.583 | 33.863 | 53.291 | 1.00 | 48.51 | 6 |
| | ATOM | 279 | O | CYS A 298 | 18.039 | 34.288 | 52.282 | 1.00 | 49.58 | 8 |
| 50 | ATOM | 280 | N | GLU A 299 | 19.144 | 34.654 | 54.202 | 1.00 | 44.17 | 7 |
| | ATOM | 281 | CA | GLU A 299 | 19.179 | 36.096 | 54.016 | 1.00 | 47.57 | 6 |
| | ATOM | 282 | CB | GLU A 299 | 19.265 | 36.833 | 55.360 | 1.00 | 49.92 | 6 |
| | ATOM | 283 | CG | GLU A 299 | 17.931 | 36.996 | 56.125 | 1.00 | 59.30 | 6 |
| | ATOM | 284 | CD | GLU A 299 | 17.613 | 35.904 | 57.095 | 1.00 | 63.80 | 6 |
| 55 | ATOM | 285 | OE1 | GLU A 299 | 16.512 | 35.952 | 57.706 | 1.00 | 69.03 | 8 |
| | ATOM | 286 | OE2 | GLU A 299 | 18.436 | 34.976 | 57.292 | 1.00 | 67.10 | 8 |
| | ATOM | 287 | C | GLU A 299 | 20.359 | 36.492 | 53.152 | 1.00 | 46.57 | 6 |
| | ATOM | 288 | O | GLU A 299 | 20.265 | 37.441 | 52.379 | 1.00 | 44.65 | 8 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 289 | N | ASP | A | 300 | 21.467 | 35.765 | 53.294 | 1.00 | 45.17 | 7 |
| | ATOM | 290 | CA | ASP | A | 300 | 22.661 | 36.042 | 52.509 | 1.00 | 43.32 | 6 |
| | ATOM | 291 | CB | ASP | A | 300 | 23.919 | 35.513 | 53.213 | 1.00 | 37.38 | 6 |
| | ATOM | 292 | CG | ASP | A | 300 | 24.223 | 36.239 | 54.473 | 1.00 | 36.23 | 6 |
| | ATOM | 293 | OD1 | ASP | A | 300 | 24.153 | 37.488 | 54.493 | 1.00 | 35.87 | 8 |
| 10 | ATOM | 294 | OD2 | ASP | A | 300 | 24.572 | 35.575 | 55.483 | 1.00 | 40.14 | 8 |
| | ATOM | 295 | C | ASP | A | 300 | 22.514 | 35.390 | 51.138 | 1.00 | 42.81 | 6 |
| | ATOM | 296 | O | ASP | A | 300 | 22.775 | 36.021 | 50.113 | 1.00 | 46.02 | 8 |
| | ATOM | 297 | N | GLN | A | 301 | 22.095 | 34.124 | 51.137 | 1.00 | 38.60 | 7 |
| | ATOM | 298 | CA | GLN | A | 301 | 21.896 | 33.390 | 49.902 | 1.00 | 40.00 | 6 |
| 15 | ATOM | 299 | CB | GLN | A | 301 | 20.991 | 32.179 | 50.137 | 1.00 | 38.59 | 6 |
| | ATOM | 300 | CG | GLN | A | 301 | 21.644 | 31.003 | 50.808 | 1.00 | 40.26 | 6 |
| | ATOM | 301 | CD | GLN | A | 301 | 20.690 | 29.824 | 50.988 | 1.00 | 44.15 | 6 |
| | ATOM | 302 | OE1 | GLN | A | 301 | 19.658 | 29.957 | 51.675 | 1.00 | 45.73 | 8 |
| | ATOM | 303 | NE2 | GLN | A | 301 | 21.027 | 28.685 | 50.394 | 1.00 | 46.13 | 7 |
| 20 | ATOM | 304 | C | GLN | A | 301 | 21.242 | 34.305 | 48.877 | 1.00 | 41.64 | 6 |
| | ATOM | 305 | O | GLN | A | 301 | 21.482 | 34.185 | 47.686 | 1.00 | 45.02 | 8 |
| | ATOM | 306 | N | ILE | A | 302 | 20.413 | 35.228 | 49.372 | 1.00 | 41.01 | 7 |
| | ATOM | 307 | CA | ILE | A | 302 | 19.726 | 36.179 | 48.511 | 1.00 | 40.23 | 6 |
| | ATOM | 308 | CB | ILE | A | 302 | 18.502 | 36.774 | 49.217 | 1.00 | 39.52 | 6 |
| 25 | ATOM | 309 | CG2 | ILE | A | 302 | 17.818 | 37.788 | 48.342 | 1.00 | 31.98 | 6 |
| | ATOM | 310 | CG1 | ILE | A | 302 | 17.502 | 35.673 | 49.581 | 1.00 | 40.77 | 6 |
| | ATOM | 311 | CD1 | ILE | A | 302 | 17.003 | 34.897 | 48.385 | 1.00 | 45.43 | 6 |
| | ATOM | 312 | C | ILE | A | 302 | 20.698 | 37.268 | 48.096 | 1.00 | 38.58 | 6 |
| | ATOM | 313 | O | ILE | A | 302 | 20.960 | 37.453 | 46.906 | 1.00 | 40.81 | 8 |
| 30 | ATOM | 314 | N | ILE | A | 303 | 21.228 | 37.972 | 49.097 | 1.00 | 37.50 | 7 |
| | ATOM | 315 | CA | ILE | A | 303 | 22.179 | 39.060 | 48.874 | 1.00 | 39.33 | 6 |
| | ATOM | 316 | CB | ILE | A | 303 | 23.023 | 39.338 | 50.109 | 1.00 | 39.06 | 6 |
| | ATOM | 317 | CG2 | ILE | A | 303 | 23.946 | 40.522 | 49.861 | 1.00 | 36.19 | 6 |
| | ATOM | 318 | CG1 | ILE | A | 303 | 22.141 | 39.653 | 51.313 | 1.00 | 40.15 | 6 |
| 35 | ATOM | 319 | CD1 | ILE | A | 303 | 22.916 | 39.806 | 52.589 | 1.00 | 36.93 | 6 |
| | ATOM | 320 | C | ILE | A | 303 | 23.093 | 38.705 | 47.722 | 1.00 | 36.49 | 6 |
| | ATOM | 321 | O | ILE | A | 303 | 23.354 | 39.509 | 46.835 | 1.00 | 36.58 | 8 |
| | ATOM | 322 | N | LEU | A | 304 | 23.580 | 37.477 | 47.762 | 1.00 | 32.91 | 7 |
| | ATOM | 323 | CA | LEU | A | 304 | 24.465 | 36.964 | 46.734 | 1.00 | 27.55 | 6 |
| 40 | ATOM | 324 | CB | LEU | A | 304 | 24.935 | 35.554 | 47.123 | 1.00 | 22.35 | 6 |
| | ATOM | 325 | CG | LEU | A | 304 | 26.150 | 35.480 | 48.029 | 1.00 | 26.88 | 6 |
| | ATOM | 326 | CD1 | LEU | A | 304 | 26.267 | 36.731 | 48.876 | 1.00 | 24.82 | 6 |
| | ATOM | 327 | CD2 | LEU | A | 304 | 26.084 | 34.226 | 48.861 | 1.00 | 23.69 | 6 |
| | ATOM | 328 | C | LEU | A | 304 | 23.764 | 36.968 | 45.389 | 1.00 | 28.05 | 6 |
| 45 | ATOM | 329 | O | LEU | A | 304 | 24.212 | 37.623 | 44.443 | 1.00 | 24.68 | 8 |
| | ATOM | 330 | N | LEU | A | 305 | 22.657 | 36.236 | 45.318 | 1.00 | 26.34 | 7 |
| | ATOM | 331 | CA | LEU | A | 305 | 21.892 | 36.147 | 44.089 | 1.00 | 30.91 | 6 |
| | ATOM | 332 | CB | LEU | A | 305 | 20.565 | 35.434 | 44.359 | 1.00 | 32.50 | 6 |
| | ATOM | 333 | CG | LEU | A | 305 | 20.637 | 33.950 | 44.635 | 1.00 | 33.36 | 6 |
| 50 | ATOM | 334 | CD1 | LEU | A | 305 | 19.247 | 33.370 | 44.779 | 1.00 | 33.87 | 6 |
| | ATOM | 335 | CD2 | LEU | A | 305 | 21.340 | 33.280 | 43.466 | 1.00 | 31.72 | 6 |
| | ATOM | 336 | C | LEU | A | 305 | 21.665 | 37.524 | 43.477 | 1.00 | 29.76 | 6 |
| | ATOM | 337 | O | LEU | A | 305 | 21.954 | 37.747 | 42.301 | 1.00 | 29.33 | 8 |
| | ATOM | 338 | N | LYS | A | 306 | 21.157 | 38.439 | 44.298 | 1.00 | 29.72 | 7 |
| 55 | ATOM | 339 | CA | LYS | A | 306 | 20.868 | 39.800 | 43.864 | 1.00 | 34.28 | 6 |
| | ATOM | 340 | CB | LYS | A | 306 | 20.293 | 40.615 | 45.026 | 1.00 | 35.98 | 6 |
| | ATOM | 341 | CG | LYS | A | 306 | 18.919 | 40.163 | 45.511 | 1.00 | 43.35 | 6 |
| | ATOM | 342 | CD | LYS | A | 306 | 18.397 | 41.127 | 46.559 | 1.00 | 51.50 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| 5 | ATOM | 343 | CE | LYS | A | 306 | 18.271 | 42.515 | 45.971 | 1.00 | 53.26 | 6 |
| | ATOM | 344 | NZ | LYS | A | 306 | 18.325 | 43.548 | 47.038 | 1.00 | 59.61 | 7 |
| | ATOM | 345 | C | LYS | A | 306 | 22.075 | 40.527 | 43.302 | 1.00 | 35.25 | 6 |
| | ATOM | 346 | O | LYS | A | 306 | 21.972 | 41.286 | 42.334 | 1.00 | 33.95 | 8 |
| | ATOM | 347 | N | GLY | A | 307 | 23.228 | 40.306 | 43.928 | 1.00 | 35.79 | 7 |
| 10 | ATOM | 348 | CA | GLY | A | 307 | 24.445 | 40.962 | 43.482 | 1.00 | 34.59 | 6 |
| | ATOM | 349 | C | GLY | A | 307 | 25.109 | 40.353 | 42.259 | 1.00 | 33.80 | 6 |
| | ATOM | 350 | O | GLY | A | 307 | 25.489 | 41.087 | 41.344 | 1.00 | 31.59 | 8 |
| | ATOM | 351 | N | CYS | A | 308 | 25.248 | 39.024 | 42.256 | 1.00 | 31.15 | 7 |
| | ATOM | 352 | CA | CYS | A | 308 | 25.899 | 38.326 | 41.174 | 1.00 | 29.04 | 6 |
| 15 | ATOM | 353 | CB | CYS | A | 308 | 26.604 | 37.089 | 41.704 | 1.00 | 27.59 | 6 |
| | ATOM | 354 | SG | CYS | A | 308 | 25.472 | 35.770 | 42.071 | 1.00 | 30.50 | 16 |
| | ATOM | 355 | C | CYS | A | 308 | 24.974 | 37.870 | 40.062 | 1.00 | 30.59 | 6 |
| | ATOM | 356 | O | CYS | A | 308 | 25.458 | 37.319 | 39.077 | 1.00 | 33.77 | 8 |
| | ATOM | 357 | N | CYS | A | 309 | 23.664 | 38.084 | 40.195 | 1.00 | 28.46 | 7 |
| 20 | ATOM | 358 | CA | CYS | A | 309 | 22.739 | 37.623 | 39.168 | 1.00 | 30.10 | 6 |
| | ATOM | 359 | CB | CYS | A | 309 | 21.311 | 38.004 | 39.490 | 1.00 | 33.43 | 6 |
| | ATOM | 360 | SG | CYS | A | 309 | 20.198 | 37.299 | 38.307 | 1.00 | 35.20 | 16 |
| | ATOM | 361 | C | CYS | A | 309 | 23.065 | 38.123 | 37.788 | 1.00 | 27.72 | 6 |
| | ATOM | 362 | O | CYS | A | 309 | 23.212 | 37.334 | 36.865 | 1.00 | 27.69 | 8 |
| 25 | ATOM | 363 | N | MET | A | 310 | 23.157 | 39.439 | 37.639 | 1.00 | 26.15 | 7 |
| | ATOM | 364 | CA | MET | A | 310 | 23.476 | 40.016 | 36.342 | 1.00 | 26.06 | 6 |
| | ATOM | 365 | CB | MET | A | 310 | 23.482 | 41.547 | 36.419 | 1.00 | 25.32 | 6 |
| | ATOM | 366 | CG | MET | A | 310 | 23.913 | 42.230 | 35.109 | 1.00 | 24.08 | 6 |
| | ATOM | 367 | SD | MET | A | 310 | 22.765 | 41.751 | 33.762 | 1.00 | 27.71 | 16 |
| 30 | ATOM | 368 | CE | MET | A | 310 | 23.650 | 42.321 | 32.270 | 1.00 | 28.50 | 6 |
| | ATOM | 369 | C | MET | A | 310 | 24.842 | 39.527 | 35.908 | 1.00 | 25.94 | 6 |
| | ATOM | 370 | O | MET | A | 310 | 25.020 | 39.076 | 34.788 | 1.00 | 28.09 | 8 |
| | ATOM | 371 | N | GLU | A | 311 | 25.800 | 39.638 | 36.826 | 1.00 | 25.39 | 7 |
| | ATOM | 372 | CA | GLU | A | 311 | 27.176 | 39.234 | 36.589 | 1.00 | 27.03 | 6 |
| 35 | ATOM | 373 | CB | GLU | A | 311 | 27.973 | 39.303 | 37.900 | 1.00 | 24.39 | 6 |
| | ATOM | 374 | CG | GLU | A | 311 | 27.842 | 40.628 | 38.668 | 1.00 | 26.00 | 6 |
| | ATOM | 375 | CD | GLU | A | 311 | 28.726 | 40.720 | 39.870 | 1.00 | 23.95 | 6 |
| | ATOM | 376 | OE1 | GLU | A | 311 | 28.891 | 39.706 | 40.588 | 1.00 | 19.72 | 8 |
| | ATOM | 377 | OE2 | GLU | A | 311 | 29.270 | 41.818 | 40.159 | 1.00 | 26.51 | 8 |
| 40 | ATOM | 378 | C | GLU | A | 311 | 27.266 | 37.827 | 35.997 | 1.00 | 27.51 | 6 |
| | ATOM | 379 | O | GLU | A | 311 | 27.956 | 37.620 | 35.014 | 1.00 | 29.67 | 8 |
| | ATOM | 380 | N | ILE | A | 312 | 26.569 | 36.866 | 36.602 | 1.00 | 26.82 | 7 |
| | ATOM | 381 | CA | ILE | A | 312 | 26.593 | 35.497 | 36.112 | 1.00 | 25.71 | 6 |
| | ATOM | 382 | CB | ILE | A | 312 | 25.991 | 34.518 | 37.123 | 1.00 | 23.35 | 6 |
| 45 | ATOM | 383 | CG2 | ILE | A | 312 | 25.917 | 33.123 | 36.533 | 1.00 | 20.27 | 6 |
| | ATOM | 384 | CG1 | ILE | A | 312 | 26.837 | 34.471 | 38.398 | 1.00 | 20.88 | 6 |
| | ATOM | 385 | CD1 | ILE | A | 312 | 26.462 | 33.342 | 39.341 | 1.00 | 18.15 | 6 |
| | ATOM | 386 | C | ILE | A | 312 | 25.871 | 35.371 | 34.791 | 1.00 | 27.91 | 6 |
| | ATOM | 387 | O | ILE | A | 312 | 26.274 | 34.593 | 33.934 | 1.00 | 28.96 | 8 |
| 50 | ATOM | 388 | N | MET | A | 313 | 24.788 | 36.130 | 34.633 | 1.00 | 27.66 | 7 |
| | ATOM | 389 | CA | MET | A | 313 | 24.013 | 36.081 | 33.395 | 1.00 | 30.18 | 6 |
| | ATOM | 390 | CB | MET | A | 313 | 22.716 | 36.888 | 33.508 | 1.00 | 36.89 | 6 |
| | ATOM | 391 | CG | MET | A | 313 | 21.608 | 36.198 | 34.305 | 1.00 | 37.95 | 6 |
| | ATOM | 392 | SD | MET | A | 313 | 19.892 | 36.817 | 34.055 | 1.00 | 42.38 | 16 |
| 55 | ATOM | 393 | CE | MET | A | 313 | 20.034 | 38.503 | 34.740 | 1.00 | 40.68 | 6 |
| | ATOM | 394 | C | MET | A | 313 | 24.834 | 36.579 | 32.222 | 1.00 | 27.43 | 6 |
| | ATOM | 395 | O | MET | A | 313 | 25.116 | 35.814 | 31.308 | 1.00 | 28.61 | 8 |
| | ATOM | 396 | N | SER | A | 314 | 25.209 | 37.859 | 32.253 | 1.00 | 24.88 | 7 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 397 | CA | SER | A | 314 | 26.005 | 38.472 | 31.197 | 1.00 | 27.98 | 6 |
| | ATOM | 398 | CB | SER | A | 314 | 26.354 | 39.914 | 31.581 | 1.00 | 29.64 | 6 |
| | ATOM | 399 | OG | SER | A | 314 | 26.956 | 39.972 | 32.858 | 1.00 | 43.44 | 8 |
| | ATOM | 400 | C | SER | A | 314 | 27.275 | 37.679 | 30.851 | 1.00 | 22.30 | 6 |
| | ATOM | 401 | O | SER | A | 314 | 27.675 | 37.629 | 29.690 | 1.00 | 24.18 | 8 |
| 10 | ATOM | 402 | N | LEU | A | 315 | 27.905 | 37.048 | 31.845 | 1.00 | 23.99 | 7 |
| | ATOM | 403 | CA | LEU | A | 315 | 29.099 | 36.261 | 31.563 | 1.00 | 25.07 | 6 |
| | ATOM | 404 | CB | LEU | A | 315 | 29.685 | 35.593 | 32.816 | 1.00 | 19.11 | 6 |
| | ATOM | 405 | CG | LEU | A | 315 | 30.675 | 34.479 | 32.505 | 1.00 | 20.39 | 6 |
| | ATOM | 406 | CD1 | LEU | A | 315 | 31.866 | 35.040 | 31.756 | 1.00 | 18.92 | 6 |
| 15 | ATOM | 407 | CD2 | LEU | A | 315 | 31.125 | 33.789 | 33.765 | 1.00 | 12.93 | 6 |
| | ATOM | 408 | C | LEU | A | 315 | 28.700 | 35.180 | 30.597 | 1.00 | 24.53 | 6 |
| | ATOM | 409 | O | LEU | A | 315 | 29.304 | 35.036 | 29.556 | 1.00 | 26.32 | 8 |
| | ATOM | 410 | N | ARG | A | 316 | 27.678 | 34.426 | 30.982 | 1.00 | 28.18 | 7 |
| | ATOM | 411 | CA | ARG | A | 316 | 27.151 | 33.312 | 30.216 | 1.00 | 27.54 | 6 |
| 20 | ATOM | 412 | CB | ARG | A | 316 | 25.915 | 32.752 | 30.928 | 1.00 | 27.39 | 6 |
| | ATOM | 413 | CG | ARG | A | 316 | 26.188 | 32.190 | 32.336 | 1.00 | 22.00 | 6 |
| | ATOM | 414 | CD | ARG | A | 316 | 24.934 | 31.526 | 32.901 | 1.00 | 18.78 | 6 |
| | ATOM | 415 | NE | ARG | A | 316 | 25.245 | 30.376 | 33.721 | 1.00 | 26.57 | 7 |
| | ATOM | 416 | CZ | ARG | A | 316 | 24.341 | 29.468 | 34.054 | 1.00 | 30.81 | 6 |
| 25 | ATOM | 417 | NH1 | ARG | A | 316 | 23.084 | 29.614 | 33.639 | 1.00 | 33.71 | 7 |
| | ATOM | 418 | NH2 | ARG | A | 316 | 24.701 | 28.416 | 34.776 | 1.00 | 33.13 | 7 |
| | ATOM | 419 | C | ARG | A | 316 | 26.774 | 33.660 | 28.794 | 1.00 | 28.09 | 6 |
| | ATOM | 420 | O | ARG | A | 316 | 26.737 | 32.792 | 27.931 | 1.00 | 32.41 | 8 |
| | ATOM | 421 | N | ALA | A | 317 | 26.484 | 34.936 | 28.571 | 1.00 | 28.36 | 7 |
| 30 | ATOM | 422 | CA | ALA | A | 317 | 26.094 | 35.411 | 27.264 | 1.00 | 26.64 | 6 |
| | ATOM | 423 | CB | ALA | A | 317 | 25.232 | 36.666 | 27.418 | 1.00 | 22.93 | 6 |
| | ATOM | 424 | C | ALA | A | 317 | 27.323 | 35.714 | 26.417 | 1.00 | 28.35 | 6 |
| | ATOM | 425 | O | ALA | A | 317 | 27.398 | 35.342 | 25.252 | 1.00 | 32.10 | 8 |
| | ATOM | 426 | N | ALA | A | 318 | 28.286 | 36.396 | 27.026 | 1.00 | 29.12 | 7 |
| 35 | ATOM | 427 | CA | ALA | A | 318 | 29.515 | 36.760 | 26.350 | 1.00 | 27.50 | 6 |
| | ATOM | 428 | CB | ALA | A | 318 | 30.434 | 37.452 | 27.333 | 1.00 | 28.39 | 6 |
| | ATOM | 429 | C | ALA | A | 318 | 30.181 | 35.502 | 25.825 | 1.00 | 28.10 | 6 |
| | ATOM | 430 | O | ALA | A | 318 | 30.600 | 35.447 | 24.678 | 1.00 | 28.18 | 8 |
| | ATOM | 431 | N | VAL | A | 319 | 30.255 | 34.491 | 26.700 | 1.00 | 29.16 | 7 |
| 40 | ATOM | 432 | CA | VAL | A | 319 | 30.880 | 33.198 | 26.393 | 1.00 | 35.24 | 6 |
| | ATOM | 433 | CB | VAL | A | 319 | 30.703 | 32.210 | 27.547 | 1.00 | 27.34 | 6 |
| | ATOM | 434 | CG1 | VAL | A | 319 | 30.895 | 32.891 | 28.858 | 1.00 | 29.96 | 6 |
| | ATOM | 435 | CG2 | VAL | A | 319 | 29.353 | 31.552 | 27.482 | 1.00 | 31.70 | 6 |
| | ATOM | 436 | C | VAL | A | 319 | 30.215 | 32.608 | 25.165 | 1.00 | 40.01 | 6 |
| 45 | ATOM | 437 | O | VAL | A | 319 | 30.640 | 31.575 | 24.680 | 1.00 | 42.70 | 8 |
| | ATOM | 438 | N | ARG | A | 320 | 29.176 | 33.284 | 24.683 | 1.00 | 38.64 | 7 |
| | ATOM | 439 | CA | ARG | A | 320 | 28.415 | 32.822 | 23.545 | 1.00 | 38.61 | 6 |
| | ATOM | 440 | CB | ARG | A | 320 | 27.031 | 32.458 | 24.043 | 1.00 | 37.26 | 6 |
| | ATOM | 441 | CG | ARG | A | 320 | 26.863 | 30.991 | 24.192 | 1.00 | 43.12 | 6 |
| 50 | ATOM | 442 | CD | ARG | A | 320 | 25.637 | 30.642 | 25.014 | 1.00 | 50.79 | 6 |
| | ATOM | 443 | NE | ARG | A | 320 | 25.258 | 29.256 | 24.770 | 1.00 | 54.71 | 7 |
| | ATOM | 444 | CZ | ARG | A | 320 | 24.331 | 28.625 | 25.501 | 1.00 | 57.89 | 6 |
| | ATOM | 445 | NH1 | ARG | A | 320 | 23.667 | 29.291 | 26.440 | 1.00 | 49.08 | 7 |
| | ATOM | 446 | NH2 | ARG | A | 320 | 23.964 | 27.385 | 25.242 | 1.00 | 59.59 | 7 |
| 55 | ATOM | 447 | C | ARG | A | 320 | 28.292 | 33.825 | 22.405 | 1.00 | 42.14 | 6 |
| | ATOM | 448 | O | ARG | A | 320 | 27.251 | 33.909 | 21.748 | 1.00 | 46.30 | 8 |
| | ATOM | 449 | N | TYR | A | 321 | 29.352 | 34.583 | 22.173 | 1.00 | 42.04 | 7 |
| | ATOM | 450 | CA | TYR | A | 321 | 29.366 | 35.555 | 21.098 | 1.00 | 42.70 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 451 | CB | TYR | A | 321 | 30.083 | 36.810 | 21.575 | 1.00 | 38.01 | 6 |
| | ATOM | 452 | CG | TYR | A | 321 | 30.601 | 37.650 | 20.448 | 1.00 | 37.94 | 6 |
| | ATOM | 453 | CD1 | TYR | A | 321 | 29.733 | 38.296 | 19.574 | 1.00 | 33.85 | 6 |
| | ATOM | 454 | CE1 | TYR | A | 321 | 30.235 | 39.037 | 18.494 | 1.00 | 34.49 | 6 |
| | ATOM | 455 | CD2 | TYR | A | 321 | 31.966 | 37.743 | 20.224 | 1.00 | 28.03 | 6 |
| 10 | ATOM | 456 | CE2 | TYR | A | 321 | 32.473 | 38.475 | 19.153 | 1.00 | 32.69 | 6 |
| | ATOM | 457 | CZ | TYR | A | 321 | 31.612 | 39.125 | 18.276 | 1.00 | 35.18 | 6 |
| | ATOM | 458 | OH | TYR | A | 321 | 32.107 | 39.866 | 17.223 | 1.00 | 39.48 | 8 |
| | ATOM | 459 | C | TYR | A | 321 | 30.085 | 35.005 | 19.877 | 1.00 | 45.51 | 6 |
| | ATOM | 460 | O | TYR | A | 321 | 31.261 | 34.697 | 19.951 | 1.00 | 48.02 | 8 |
| 15 | ATOM | 461 | N | ASP | A | 322 | 29.354 | 34.879 | 18.773 | 1.00 | 44.56 | 7 |
| | ATOM | 462 | CA | ASP | A | 322 | 29.912 | 34.400 | 17.502 | 1.00 | 45.86 | 6 |
| | ATOM | 463 | CB | ASP | A | 322 | 28.804 | 33.670 | 16.736 | 1.00 | 46.64 | 6 |
| | ATOM | 464 | CG | ASP | A | 322 | 29.050 | 33.608 | 15.255 | 1.00 | 40.00 | 6 |
| | ATOM | 465 | OD1 | ASP | A | 322 | 30.010 | 34.256 | 14.768 | 1.00 | 40.00 | 8 |
| 20 | ATOM | 466 | OD2 | ASP | A | 322 | 28.262 | 32.929 | 14.536 | 1.00 | 40.00 | 8 |
| | ATOM | 467 | C | ASP | A | 322 | 30.460 | 35.629 | 16.755 | 1.00 | 45.82 | 6 |
| | ATOM | 468 | O | ASP | A | 322 | 29.678 | 36.464 | 16.271 | 1.00 | 45.38 | 8 |
| | ATOM | 469 | N | PRO | A | 323 | 31.800 | 35.735 | 16.584 | 1.00 | 46.53 | 7 |
| | ATOM | 470 | CD | PRO | A | 323 | 32.774 | 34.719 | 16.991 | 1.00 | 47.16 | 6 |
| 25 | ATOM | 471 | CA | PRO | A | 323 | 32.424 | 36.889 | 15.890 | 1.00 | 46.63 | 6 |
| | ATOM | 472 | CB | PRO | A | 323 | 33.921 | 36.603 | 15.936 | 1.00 | 43.95 | 6 |
| | ATOM | 473 | CG | PRO | A | 323 | 34.099 | 35.303 | 16.582 | 1.00 | 43.93 | 6 |
| | ATOM | 474 | C | PRO | A | 323 | 31.953 | 37.087 | 14.453 | 1.00 | 48.34 | 6 |
| | ATOM | 475 | O | PRO | A | 323 | 31.797 | 38.210 | 13.960 | 1.00 | 50.84 | 8 |
| 30 | ATOM | 476 | N | GLU | A | 324 | 31.778 | 35.970 | 13.752 | 1.00 | 52.39 | 7 |
| | ATOM | 477 | CA | GLU | A | 324 | 31.339 | 35.968 | 12.370 | 1.00 | 55.85 | 6 |
| | ATOM | 478 | CB | GLU | A | 324 | 31.035 | 34.528 | 11.965 | 1.00 | 55.54 | 6 |
| | ATOM | 479 | CG | GLU | A | 324 | 32.224 | 33.584 | 12.104 | 1.00 | 40.00 | 6 |
| | ATOM | 480 | CD | GLU | A | 324 | 33.432 | 34.023 | 11.310 | 1.00 | 40.00 | 6 |
| 35 | ATOM | 481 | OE1 | GLU | A | 324 | 33.350 | 35.040 | 10.555 | 1.00 | 40.00 | 8 |
| | ATOM | 482 | OE2 | GLU | A | 324 | 34.506 | 33.356 | 11.415 | 1.00 | 40.00 | 8 |
| | ATOM | 483 | C | GLU | A | 324 | 30.077 | 36.798 | 12.277 | 1.00 | 54.94 | 6 |
| | ATOM | 484 | O | GLU | A | 324 | 30.070 | 37.892 | 11.730 | 1.00 | 59.81 | 8 |
| | ATOM | 485 | N | SER | A | 325 | 29.009 | 36.212 | 12.810 | 1.00 | 52.95 | 7 |
| 40 | ATOM | 486 | CA | SER | A | 325 | 27.695 | 36.812 | 12.839 | 1.00 | 50.10 | 6 |
| | ATOM | 487 | CB | SER | A | 325 | 26.701 | 35.797 | 13.402 | 1.00 | 48.23 | 6 |
| | ATOM | 488 | OG | SER | A | 325 | 27.183 | 35.239 | 14.615 | 1.00 | 48.71 | 8 |
| | ATOM | 489 | C | SER | A | 325 | 27.651 | 38.093 | 13.659 | 1.00 | 50.61 | 6 |
| | ATOM | 490 | O | SER | A | 325 | 26.885 | 38.992 | 13.354 | 1.00 | 52.19 | 8 |
| 45 | ATOM | 491 | N | GLU | A | 326 | 28.495 | 38.168 | 14.687 | 1.00 | 45.64 | 7 |
| | ATOM | 492 | CA | GLU | A | 326 | 28.567 | 39.341 | 15.546 | 1.00 | 43.35 | 6 |
| | ATOM | 493 | CB | GLU | A | 326 | 28.830 | 40.608 | 14.711 | 1.00 | 42.74 | 6 |
| | ATOM | 494 | CG | GLU | A | 326 | 30.148 | 40.606 | 13.945 | 1.00 | 50.32 | 6 |
| | ATOM | 495 | CD | GLU | A | 326 | 30.451 | 41.925 | 13.313 | 1.00 | 56.34 | 6 |
| 50 | ATOM | 496 | OE1 | GLU | A | 326 | 31.509 | 42.046 | 12.649 | 1.00 | 59.31 | 8 |
| | ATOM | 497 | OE2 | GLU | A | 326 | 29.656 | 42.890 | 13.452 | 1.00 | 55.74 | 8 |
| | ATOM | 498 | C | GLU | A | 326 | 27.288 | 39.526 | 16.340 | 1.00 | 40.23 | 6 |
| | ATOM | 499 | O | GLU | A | 326 | 26.695 | 40.603 | 16.340 | 1.00 | 40.44 | 8 |
| | ATOM | 500 | N | THR | A | 327 | 26.888 | 38.474 | 17.051 | 1.00 | 35.90 | 7 |
| 55 | ATOM | 501 | CA | THR | A | 327 | 25.663 | 38.506 | 17.860 | 1.00 | 37.29 | 6 |
| | ATOM | 502 | CB | THR | A | 327 | 24.466 | 38.057 | 17.024 | 1.00 | 37.63 | 6 |
| | ATOM | 503 | OG1 | THR | A | 327 | 24.661 | 36.709 | 16.580 | 1.00 | 38.12 | 8 |
| | ATOM | 504 | CG2 | THR | A | 327 | 24.269 | 38.965 | 15.810 | 1.00 | 39.90 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| 5 | ATOM | 505 | C | THR | A | 327 | 25.767 | 37.562 | 19.038 | 1.00 | 39.49 | 6 |
| | ATOM | 506 | O | THR | A | 327 | 26.284 | 36.458 | 18.903 | 1.00 | 40.50 | 8 |
| | ATOM | 507 | N | LEU | A | 328 | 25.250 | 37.987 | 20.184 | 1.00 | 36.64 | 7 |
| | ATOM | 508 | CA | LEU | A | 328 | 25.264 | 37.141 | 21.381 | 1.00 | 37.73 | 6 |
| | ATOM | 509 | CB | LEU | A | 328 | 25.148 | 37.999 | 22.650 | 1.00 | 37.78 | 6 |
| 10 | ATOM | 510 | CG | LEU | A | 328 | 26.102 | 39.150 | 22.843 | 1.00 | 36.26 | 6 |
| | ATOM | 511 | CD1 | LEU | A | 328 | 26.066 | 39.623 | 24.272 | 1.00 | 36.56 | 6 |
| | ATOM | 512 | CD2 | LEU | A | 328 | 27.481 | 38.688 | 22.500 | 1.00 | 39.85 | 6 |
| | ATOM | 513 | C | LEU | A | 328 | 24.063 | 36.220 | 21.244 | 1.00 | 37.27 | 6 |
| | ATOM | 514 | O | LEU | A | 328 | 23.306 | 36.337 | 20.279 | 1.00 | 34.96 | 8 |
| 15 | ATOM | 515 | N | THR | A | 329 | 23.891 | 35.317 | 22.205 | 1.00 | 39.73 | 7 |
| | ATOM | 516 | CA | THR | A | 329 | 22.785 | 34.376 | 22.180 | 1.00 | 40.81 | 6 |
| | ATOM | 517 | CB | THR | A | 329 | 23.241 | 32.991 | 21.699 | 1.00 | 42.67 | 6 |
| | ATOM | 518 | OG1 | THR | A | 329 | 23.879 | 33.103 | 20.421 | 1.00 | 42.52 | 8 |
| | ATOM | 519 | CG2 | THR | A | 329 | 22.026 | 32.057 | 21.589 | 1.00 | 43.52 | 6 |
| 20 | ATOM | 520 | C | THR | A | 329 | 22.168 | 34.245 | 23.548 | 1.00 | 44.31 | 6 |
| | ATOM | 521 | O | THR | A | 329 | 22.526 | 33.370 | 24.320 | 1.00 | 43.72 | 8 |
| | ATOM | 522 | N | LEU | A | 330 | 21.237 | 35.149 | 23.830 | 1.00 | 44.62 | 7 |
| | ATOM | 523 | CA | LEU | A | 330 | 20.532 | 35.170 | 25.111 | 1.00 | 45.09 | 6 |
| | ATOM | 524 | CB | LEU | A | 330 | 19.677 | 36.444 | 25.195 | 1.00 | 44.66 | 6 |
| 25 | ATOM | 525 | CG | LEU | A | 330 | 20.436 | 37.750 | 25.259 | 1.00 | 51.06 | 6 |
| | ATOM | 526 | CD1 | LEU | A | 330 | 21.405 | 37.831 | 24.104 | 1.00 | 48.58 | 6 |
| | ATOM | 527 | CD2 | LEU | A | 330 | 19.466 | 38.909 | 25.238 | 1.00 | 45.18 | 6 |
| | ATOM | 528 | C | LEU | A | 330 | 19.656 | 33.919 | 25.301 | 1.00 | 48.06 | 6 |
| | ATOM | 529 | O | LEU | A | 330 | 19.049 | 33.422 | 24.359 | 1.00 | 49.33 | 8 |
| 30 | ATOM | 530 | N | ASN | A | 331 | 19.618 | 33.431 | 26.540 | 1.00 | 52.20 | 7 |
| | ATOM | 531 | CA | ASN | A | 331 | 18.842 | 32.256 | 26.913 | 1.00 | 54.41 | 6 |
| | ATOM | 532 | CB | ASN | A | 331 | 17.361 | 32.628 | 27.009 | 1.00 | 54.94 | 6 |
| | ATOM | 533 | CG | ASN | A | 331 | 16.724 | 32.112 | 28.269 | 1.00 | 60.35 | 6 |
| | ATOM | 534 | OD1 | ASN | A | 331 | 17.124 | 32.505 | 29.383 | 1.00 | 61.84 | 8 |
| 35 | ATOM | 535 | ND2 | ASN | A | 331 | 15.750 | 31.238 | 28.117 | 1.00 | 65.92 | 7 |
| | ATOM | 536 | C | ASN | A | 331 | 19.016 | 31.108 | 25.934 | 1.00 | 58.00 | 6 |
| | ATOM | 537 | O | ASN | A | 331 | 18.243 | 30.157 | 25.941 | 1.00 | 60.17 | 8 |
| | ATOM | 538 | N | GLY | A | 332 | 20.063 | 31.196 | 25.114 | 1.00 | 58.45 | 7 |
| | ATOM | 539 | CA | GLY | A | 332 | 20.341 | 30.161 | 24.131 | 1.00 | 58.55 | 6 |
| 40 | ATOM | 540 | C | GLY | A | 332 | 19.316 | 30.016 | 23.021 | 1.00 | 59.79 | 6 |
| | ATOM | 541 | O | GLY | A | 332 | 19.413 | 29.094 | 22.213 | 1.00 | 61.32 | 8 |
| | ATOM | 542 | N | GLU | A | 333 | 18.346 | 30.929 | 22.983 | 1.00 | 60.28 | 7 |
| | ATOM | 543 | CA | GLU | A | 333 | 17.294 | 30.883 | 21.985 | 1.00 | 59.13 | 6 |
| | ATOM | 544 | CB | GLU | A | 333 | 15.919 | 30.875 | 22.662 | 1.00 | 62.40 | 6 |
| 45 | ATOM | 545 | CG | GLU | A | 333 | 15.667 | 29.750 | 23.658 | 1.00 | 75.69 | 6 |
| | ATOM | 546 | CD | GLU | A | 333 | 14.341 | 29.865 | 24.346 | 1.00 | 80.41 | 6 |
| | ATOM | 547 | OE1 | GLU | A | 333 | 14.052 | 30.932 | 24.945 | 1.00 | 79.98 | 8 |
| | ATOM | 548 | OE2 | GLU | A | 333 | 13.549 | 28.884 | 24.329 | 1.00 | 83.81 | 8 |
| | ATOM | 549 | C | GLU | A | 333 | 17.356 | 32.090 | 21.073 | 1.00 | 57.18 | 6 |
| 50 | ATOM | 550 | O | GLU | A | 333 | 17.239 | 31.969 | 19.852 | 1.00 | 57.50 | 8 |
| | ATOM | 551 | N | MET | A | 334 | 17.512 | 33.258 | 21.696 | 1.00 | 55.20 | 7 |
| | ATOM | 552 | CA | MET | A | 334 | 17.561 | 34.529 | 20.980 | 1.00 | 50.85 | 6 |
| | ATOM | 553 | CB | MET | A | 334 | 16.751 | 35.556 | 21.763 | 1.00 | 48.70 | 6 |
| | ATOM | 554 | CG | MET | A | 334 | 16.859 | 36.947 | 21.212 | 1.00 | 45.39 | 6 |
| 55 | ATOM | 555 | SD | MET | A | 334 | 15.881 | 38.186 | 22.127 | 1.00 | 44.56 | 16 |
| | ATOM | 556 | CE | MET | A | 334 | 14.229 | 37.371 | 22.113 | 1.00 | 45.25 | 6 |
| | ATOM | 557 | C | MET | A | 334 | 18.956 | 35.087 | 20.713 | 1.00 | 51.59 | 6 |
| | ATOM | 558 | O | MET | A | 334 | 19.739 | 35.268 | 21.633 | 1.00 | 52.52 | 8 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 559 | N | ALA | A | 335 | 19.234 | 35.371 | 19.444 | 1.00 | 51.00 | 7 |
| | ATOM | 560 | CA | ALA | A | 335 | 20.520 | 35.932 | 19.039 | 1.00 | 48.98 | 6 |
| | ATOM | 561 | CB | ALA | A | 335 | 20.997 | 35.254 | 17.768 | 1.00 | 47.86 | 6 |
| | ATOM | 562 | C | ALA | A | 335 | 20.342 | 37.420 | 18.805 | 1.00 | 51.01 | 6 |
| | ATOM | 563 | O | ALA | A | 335 | 19.594 | 37.830 | 17.919 | 1.00 | 51.61 | 8 |
| 10 | ATOM | 564 | N | VAL | A | 336 | 21.024 | 38.232 | 19.612 | 1.00 | 46.62 | 7 |
| | ATOM | 565 | CA | VAL | A | 336 | 20.910 | 39.699 | 19.502 | 1.00 | 42.35 | 6 |
| | ATOM | 566 | CB | VAL | A | 336 | 20.517 | 40.325 | 20.840 | 1.00 | 42.41 | 6 |
| | ATOM | 567 | CG1 | VAL | A | 336 | 19.242 | 39.691 | 21.361 | 1.00 | 42.00 | 6 |
| | ATOM | 568 | CG2 | VAL | A | 336 | 21.639 | 40.211 | 21.852 | 1.00 | 40.32 | 6 |
| 15 | ATOM | 569 | C | VAL | A | 336 | 22.204 | 40.321 | 19.036 | 1.00 | 45.33 | 6 |
| | ATOM | 570 | O | VAL | A | 336 | 23.263 | 39.691 | 19.025 | 1.00 | 47.42 | 8 |
| | ATOM | 571 | N | THR | A | 337 | 22.090 | 41.590 | 18.668 | 1.00 | 41.60 | 7 |
| | ATOM | 572 | CA | THR | A | 337 | 23.230 | 42.377 | 18.175 | 1.00 | 39.69 | 6 |
| | ATOM | 573 | CB | THR | A | 337 | 22.882 | 43.061 | 16.852 | 1.00 | 41.35 | 6 |
| 20 | ATOM | 574 | OG1 | THR | A | 337 | 21.987 | 44.157 | 17.080 | 1.00 | 49.35 | 8 |
| | ATOM | 575 | CG2 | THR | A | 337 | 22.216 | 42.067 | 15.904 | 1.00 | 40.38 | 6 |
| | ATOM | 576 | C | THR | A | 337 | 23.588 | 43.481 | 19.159 | 1.00 | 37.88 | 6 |
| | ATOM | 577 | O | THR | A | 337 | 22.734 | 43.989 | 19.892 | 1.00 | 34.06 | 8 |
| | ATOM | 578 | N | ARG | A | 338 | 24.865 | 43.849 | 19.138 | 1.00 | 37.61 | 7 |
| 25 | ATOM | 579 | CA | ARG | A | 338 | 25.388 | 44.919 | 19.984 | 1.00 | 38.68 | 6 |
| | ATOM | 580 | CB | ARG | A | 338 | 26.669 | 45.479 | 19.351 | 1.00 | 35.95 | 6 |
| | ATOM | 581 | CG | ARG | A | 338 | 27.250 | 46.713 | 20.038 | 1.00 | 38.83 | 6 |
| | ATOM | 582 | CD | ARG | A | 338 | 28.443 | 47.254 | 19.247 | 1.00 | 35.88 | 6 |
| | ATOM | 583 | NE | ARG | A | 338 | 29.559 | 46.320 | 19.175 | 1.00 | 37.42 | 7 |
| 30 | ATOM | 584 | CZ | ARG | A | 338 | 30.449 | 46.122 | 20.145 | 1.00 | 30.20 | 6 |
| | ATOM | 585 | NH1 | ARG | A | 338 | 30.338 | 46.791 | 21.295 | 1.00 | 27.98 | 7 |
| | ATOM | 586 | NH2 | ARG | A | 338 | 31.433 | 45.240 | 19.954 | 1.00 | 27.40 | 7 |
| | ATOM | 587 | C | ARG | A | 338 | 24.333 | 46.010 | 20.085 | 1.00 | 38.09 | 6 |
| | ATOM | 588 | O | ARG | A | 338 | 23.894 | 46.397 | 21.169 | 1.00 | 34.12 | 8 |
| 35 | ATOM | 589 | N | GLY | A | 339 | 23.915 | 46.496 | 18.922 | 1.00 | 41.25 | 7 |
| | ATOM | 590 | CA | GLY | A | 339 | 22.918 | 47.547 | 18.890 | 1.00 | 41.35 | 6 |
| | ATOM | 591 | C | GLY | A | 339 | 21.692 | 47.140 | 19.672 | 1.00 | 41.23 | 6 |
| | ATOM | 592 | O | GLY | A | 339 | 21.445 | 47.671 | 20.750 | 1.00 | 38.30 | 8 |
| | ATOM | 593 | N | GLN | A | 340 | 20.924 | 46.203 | 19.105 | 1.00 | 38.58 | 7 |
| 40 | ATOM | 594 | CA | GLN | A | 340 | 19.701 | 45.700 | 19.729 | 1.00 | 40.79 | 6 |
| | ATOM | 595 | CB | GLN | A | 340 | 19.436 | 44.260 | 19.253 | 1.00 | 40.82 | 6 |
| | ATOM | 596 | CG | GLN | A | 340 | 19.087 | 44.146 | 17.767 | 1.00 | 41.10 | 6 |
| | ATOM | 597 | CD | GLN | A | 340 | 18.876 | 42.705 | 17.305 | 1.00 | 48.84 | 6 |
| | ATOM | 598 | OE1 | GLN | A | 340 | 19.826 | 41.888 | 17.309 | 1.00 | 50.53 | 8 |
| 45 | ATOM | 599 | NE2 | GLN | A | 340 | 17.650 | 42.393 | 16.907 | 1.00 | 54.25 | 7 |
| | ATOM | 600 | C | GLN | A | 340 | 19.779 | 45.750 | 21.263 | 1.00 | 41.50 | 6 |
| | ATOM | 601 | O | GLN | A | 340 | 18.998 | 46.444 | 21.923 | 1.00 | 42.72 | 8 |
| | ATOM | 602 | N | LEU | A | 341 | 20.758 | 45.026 | 21.806 | 1.00 | 42.00 | 7 |
| | ATOM | 603 | CA | LEU | A | 341 | 20.952 | 44.947 | 23.243 | 1.00 | 38.10 | 6 |
| 50 | ATOM | 604 | CB | LEU | A | 341 | 22.209 | 44.145 | 23.575 | 1.00 | 36.66 | 6 |
| | ATOM | 605 | CG | LEU | A | 341 | 22.361 | 43.804 | 25.029 | 1.00 | 39.94 | 6 |
| | ATOM | 606 | CD1 | LEU | A | 341 | 21.219 | 42.884 | 25.410 | 1.00 | 34.98 | 6 |
| | ATOM | 607 | CD2 | LEU | A | 341 | 23.685 | 43.128 | 25.284 | 1.00 | 40.95 | 6 |
| | ATOM | 608 | C | LEU | A | 341 | 21.072 | 46.321 | 23.860 | 1.00 | 36.37 | 6 |
| 55 | ATOM | 609 | O | LEU | A | 341 | 20.484 | 46.588 | 24.892 | 1.00 | 37.89 | 8 |
| | ATOM | 610 | N | LYS | A | 342 | 21.848 | 47.184 | 23.209 | 1.00 | 33.29 | 7 |
| | ATOM | 611 | CA | LYS | A | 342 | 22.089 | 48.546 | 23.679 | 1.00 | 35.17 | 6 |
| | ATOM | 612 | CB | LYS | A | 342 | 23.057 | 49.242 | 22.721 | 1.00 | 34.97 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 613 | CG | LYS | A | 342 | 23.655 | 50.536 | 23.240 | 1.00 | 40.00 | 6 |
| | ATOM | 614 | CD | LYS | A | 342 | 24.673 | 51.109 | 22.245 | 1.00 | 34.48 | 6 |
| | ATOM | 615 | CE | LYS | A | 342 | 25.514 | 52.229 | 22.873 | 1.00 | 37.54 | 6 |
| | ATOM | 616 | NZ | LYS | A | 342 | 26.655 | 52.634 | 21.987 | 1.00 | 42.32 | 7 |
| | ATOM | 617 | C | LYS | A | 342 | 20.796 | 49.349 | 23.774 | 1.00 | 38.29 | 8 |
| 10 | ATOM | 618 | O | LYS | A | 342 | 20.345 | 49.711 | 24.861 | 1.00 | 36.23 | 8 |
| | ATOM | 619 | N | ASN | A | 343 | 20.223 | 49.622 | 22.603 | 1.00 | 39.25 | 7 |
| | ATOM | 620 | CA | ASN | A | 343 | 18.993 | 50.385 | 22.485 | 1.00 | 40.19 | 6 |
| | ATOM | 621 | CB | ASN | A | 343 | 18.521 | 50.373 | 21.033 | 1.00 | 37.96 | 6 |
| | ATOM | 622 | CG | ASN | A | 343 | 19.664 | 50.550 | 20.052 | 1.00 | 39.22 | 6 |
| 15 | ATOM | 623 | OD1 | ASN | A | 343 | 20.428 | 51.537 | 20.125 | 1.00 | 42.37 | 8 |
| | ATOM | 624 | ND2 | ASN | A | 343 | 19.773 | 49.612 | 19.125 | 1.00 | 42.19 | 7 |
| | ATOM | 625 | C | ASN | A | 343 | 17.928 | 49.748 | 23.375 | 1.00 | 40.12 | 6 |
| | ATOM | 626 | O | ASN | A | 343 | 17.010 | 50.417 | 23.859 | 1.00 | 36.01 | 8 |
| | ATOM | 627 | N | GLY | A | 344 | 18.073 | 48.433 | 23.568 | 1.00 | 40.95 | 7 |
| 20 | ATOM | 628 | CA | GLY | A | 344 | 17.152 | 47.670 | 24.394 | 1.00 | 39.25 | 6 |
| | ATOM | 629 | C | GLY | A | 344 | 17.039 | 48.092 | 25.842 | 1.00 | 38.26 | 6 |
| | ATOM | 630 | O | GLY | A | 344 | 16.072 | 47.724 | 26.512 | 1.00 | 35.69 | 8 |
| | ATOM | 631 | N | GLY | A | 345 | 18.017 | 48.857 | 26.329 | 1.00 | 35.89 | 7 |
| | ATOM | 632 | CA | GLY | A | 345 | 17.964 | 49.301 | 27.706 | 1.00 | 34.00 | 6 |
| 25 | ATOM | 633 | C | GLY | A | 345 | 19.273 | 49.199 | 28.443 | 1.00 | 38.64 | 6 |
| | ATOM | 634 | O | GLY | A | 345 | 19.469 | 49.888 | 29.441 | 1.00 | 38.14 | 8 |
| | ATOM | 635 | N | LEU | A | 346 | 20.170 | 48.337 | 27.973 | 1.00 | 39.52 | 7 |
| | ATOM | 636 | CA | LEU | A | 346 | 21.444 | 48.180 | 28.649 | 1.00 | 36.05 | 6 |
| | ATOM | 637 | CB | LEU | A | 346 | 22.124 | 46.876 | 28.209 | 1.00 | 35.72 | 6 |
| 30 | ATOM | 638 | CG | LEU | A | 346 | 21.355 | 45.617 | 28.501 | 1.00 | 34.89 | 6 |
| | ATOM | 639 | CD1 | LEU | A | 346 | 22.295 | 44.413 | 28.422 | 1.00 | 44.09 | 6 |
| | ATOM | 640 | CD2 | LEU | A | 346 | 20.786 | 45.721 | 29.902 | 1.00 | 34.84 | 6 |
| | ATOM | 641 | C | LEU | A | 346 | 22.358 | 49.361 | 28.396 | 1.00 | 33.52 | 6 |
| | ATOM | 642 | O | LEU | A | 346 | 23.267 | 49.653 | 29.178 | 1.00 | 35.58 | 8 |
| 35 | ATOM | 643 | N | GLY | A | 347 | 22.087 | 50.056 | 27.295 | 1.00 | 30.47 | 7 |
| | ATOM | 644 | CA | GLY | A | 347 | 22.909 | 51.192 | 26.931 | 1.00 | 33.01 | 6 |
| | ATOM | 645 | C | GLY | A | 347 | 24.360 | 50.768 | 26.747 | 1.00 | 30.72 | 6 |
| | ATOM | 646 | O | GLY | A | 347 | 24.669 | 49.775 | 26.082 | 1.00 | 30.89 | 8 |
| | ATOM | 647 | N | VAL | A | 348 | 25.244 | 51.556 | 27.355 | 1.00 | 31.30 | 7 |
| 40 | ATOM | 648 | CA | VAL | A | 348 | 26.671 | 51.325 | 27.286 | 1.00 | 31.27 | 6 |
| | ATOM | 649 | CB | VAL | A | 348 | 27.441 | 52.294 | 28.184 | 1.00 | 31.66 | 6 |
| | ATOM | 650 | CG1 | VAL | A | 348 | 27.067 | 52.107 | 29.631 | 1.00 | 20.19 | 6 |
| | ATOM | 651 | CG2 | VAL | A | 348 | 28.931 | 52.138 | 27.986 | 1.00 | 24.77 | 6 |
| | ATOM | 652 | C | VAL | A | 348 | 27.063 | 49.892 | 27.678 | 1.00 | 33.84 | 6 |
| 45 | ATOM | 653 | O | VAL | A | 348 | 28.095 | 49.392 | 27.225 | 1.00 | 29.99 | 8 |
| | ATOM | 654 | N | VAL | A | 349 | 26.253 | 49.227 | 28.514 | 1.00 | 33.31 | 7 |
| | ATOM | 655 | CA | VAL | A | 349 | 26.568 | 47.881 | 28.906 | 1.00 | 32.23 | 6 |
| | ATOM | 656 | CB | VAL | A | 349 | 25.581 | 47.259 | 29.858 | 1.00 | 32.59 | 6 |
| | ATOM | 657 | CG1 | VAL | A | 349 | 25.865 | 45.795 | 29.985 | 1.00 | 33.68 | 6 |
| 50 | ATOM | 658 | CG2 | VAL | A | 349 | 25.687 | 47.899 | 31.213 | 1.00 | 32.30 | 6 |
| | ATOM | 659 | C | VAL | A | 349 | 26.706 | 46.985 | 27.726 | 1.00 | 34.91 | 6 |
| | ATOM | 660 | O | VAL | A | 349 | 27.583 | 46.136 | 27.735 | 1.00 | 33.73 | 8 |
| | ATOM | 661 | N | SER | A | 350 | 25.875 | 47.134 | 26.702 | 1.00 | 32.81 | 7 |
| | ATOM | 662 | CA | SER | A | 350 | 26.001 | 46.252 | 25.556 | 1.00 | 30.10 | 6 |
| 55 | ATOM | 663 | CB | SER | A | 350 | 25.119 | 46.665 | 24.411 | 1.00 | 24.95 | 6 |
| | ATOM | 664 | OG | SER | A | 350 | 25.209 | 45.675 | 23.394 | 1.00 | 23.16 | 8 |
| | ATOM | 665 | C | SER | A | 350 | 27.445 | 46.257 | 25.129 | 1.00 | 31.59 | 6 |
| | ATOM | 666 | O | SER | A | 350 | 28.116 | 45.244 | 25.284 | 1.00 | 37.62 | 8 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 667 | N | ASP | A | 351 | 27.945 | 47.367 | 24.591 | 1.00 | 28.60 | 7 |
| | ATOM | 668 | CA | ASP | A | 351 | 29.351 | 47.437 | 24.183 | 1.00 | 29.82 | 6 |
| | ATOM | 669 | CB | ASP | A | 351 | 29.808 | 48.891 | 24.105 | 1.00 | 27.49 | 6 |
| | ATOM | 670 | CG | ASP | A | 351 | 28.875 | 49.744 | 23.303 | 1.00 | 30.22 | 6 |
| | ATOM | 671 | OD1 | ASP | A | 351 | 28.055 | 50.483 | 23.909 | 1.00 | 32.61 | 8 |
| 10 | ATOM | 672 | OD2 | ASP | A | 351 | 28.942 | 49.714 | 22.044 | 1.00 | 30.02 | 8 |
| | ATOM | 673 | C | ASP | A | 351 | 30.173 | 46.653 | 25.231 | 1.00 | 30.63 | 6 |
| | ATOM | 674 | O | ASP | A | 351 | 30.981 | 45.792 | 24.903 | 1.00 | 29.54 | 8 |
| | ATOM | 675 | N | ALA | A | 352 | 29.939 | 46.949 | 26.503 | 1.00 | 25.33 | 7 |
| | ATOM | 676 | CA | ALA | A | 352 | 30.623 | 46.280 | 27.602 | 1.00 | 28.59 | 6 |
| 15 | ATOM | 677 | CB | ALA | A | 352 | 30.072 | 46.799 | 28.922 | 1.00 | 20.95 | 6 |
| | ATOM | 678 | C | ALA | A | 352 | 30.492 | 44.756 | 27.527 | 1.00 | 29.69 | 6 |
| | ATOM | 679 | O | ALA | A | 352 | 31.481 | 44.054 | 27.587 | 1.00 | 30.36 | 8 |
| | ATOM | 680 | N | ILE | A | 353 | 29.260 | 44.260 | 27.413 | 1.00 | 27.63 | 7 |
| | ATOM | 681 | CA | ILE | A | 353 | 29.003 | 42.832 | 27.326 | 1.00 | 27.55 | 6 |
| 20 | ATOM | 682 | CB | ILE | A | 353 | 27.512 | 42.528 | 27.429 | 1.00 | 28.04 | 6 |
| | ATOM | 683 | CG2 | ILE | A | 353 | 27.269 | 41.042 | 27.289 | 1.00 | 23.68 | 6 |
| | ATOM | 684 | CG1 | ILE | A | 353 | 26.955 | 42.965 | 28.789 | 1.00 | 27.33 | 6 |
| | ATOM | 685 | CD1 | ILE | A | 353 | 25.452 | 42.688 | 28.944 | 1.00 | 26.23 | 6 |
| | ATOM | 686 | C | ILE | A | 353 | 29.534 | 42.207 | 26.054 | 1.00 | 30.88 | 6 |
| 25 | ATOM | 687 | O | ILE | A | 353 | 30.007 | 41.076 | 26.068 | 1.00 | 31.22 | 8 |
| | ATOM | 688 | N | PHE | A | 354 | 29.426 | 42.917 | 24.939 | 1.00 | 29.86 | 7 |
| | ATOM | 689 | CA | PHE | A | 354 | 29.922 | 42.369 | 23.686 | 1.00 | 31.08 | 6 |
| | ATOM | 690 | CB | PHE | A | 354 | 29.371 | 43.146 | 22.487 | 1.00 | 28.80 | 6 |
| | ATOM | 691 | CG | PHE | A | 354 | 28.029 | 42.643 | 21.988 | 1.00 | 28.80 | 6 |
| 30 | ATOM | 692 | CD1 | PHE | A | 354 | 26.872 | 42.842 | 22.724 | 1.00 | 30.96 | 6 |
| | ATOM | 693 | CD2 | PHE | A | 354 | 27.950 | 41.953 | 20.783 | 1.00 | 29.45 | 6 |
| | ATOM | 694 | CE1 | PHE | A | 354 | 25.657 | 42.360 | 22.250 | 1.00 | 27.12 | 6 |
| | ATOM | 695 | CE2 | PHE | A | 354 | 26.738 | 41.470 | 20.305 | 1.00 | 25.19 | 6 |
| | ATOM | 696 | CZ | PHE | A | 354 | 25.590 | 41.672 | 21.038 | 1.00 | 28.09 | 6 |
| 35 | ATOM | 697 | C | PHE | A | 354 | 31.444 | 42.399 | 23.682 | 1.00 | 29.17 | 6 |
| | ATOM | 698 | O | PHE | A | 354 | 32.087 | 41.389 | 23.398 | 1.00 | 32.62 | 8 |
| | ATOM | 699 | N | ASP | A | 355 | 32.013 | 43.569 | 23.980 | 1.00 | 23.86 | 7 |
| | ATOM | 700 | CA | ASP | A | 355 | 33.466 | 43.739 | 24.030 | 1.00 | 25.34 | 6 |
| | ATOM | 701 | CB | ASP | A | 355 | 33.820 | 45.053 | 24.737 | 1.00 | 21.41 | 6 |
| 40 | ATOM | 702 | CG | ASP | A | 355 | 33.841 | 46.226 | 23.809 | 1.00 | 32.08 | 6 |
| | ATOM | 703 | OD1 | ASP | A | 355 | 32.979 | 46.322 | 22.902 | 1.00 | 33.58 | 8 |
| | ATOM | 704 | OD2 | ASP | A | 355 | 34.711 | 47.117 | 23.968 | 1.00 | 33.20 | 8 |
| | ATOM | 705 | C | ASP | A | 355 | 34.074 | 42.559 | 24.781 | 1.00 | 27.86 | 6 |
| | ATOM | 706 | O | ASP | A | 355 | 35.131 | 42.053 | 24.410 | 1.00 | 32.42 | 8 |
| 45 | ATOM | 707 | N | LEU | A | 356 | 33.387 | 42.128 | 25.843 | 1.00 | 26.84 | 7 |
| | ATOM | 708 | CA | LEU | A | 356 | 33.845 | 40.993 | 26.642 | 1.00 | 28.66 | 6 |
| | ATOM | 709 | CB | LEU | A | 356 | 32.893 | 40.747 | 27.825 | 1.00 | 25.37 | 6 |
| | ATOM | 710 | CG | LEU | A | 356 | 33.235 | 39.608 | 28.755 | 1.00 | 27.61 | 6 |
| | ATOM | 711 | CD1 | LEU | A | 356 | 34.538 | 39.917 | 29.451 | 1.00 | 25.43 | 6 |
| 50 | ATOM | 712 | CD2 | LEU | A | 356 | 32.149 | 39.414 | 29.765 | 1.00 | 27.49 | 6 |
| | ATOM | 713 | C | LEU | A | 356 | 33.849 | 39.779 | 25.723 | 1.00 | 30.44 | 6 |
| | ATOM | 714 | O | LEU | A | 356 | 34.884 | 39.160 | 25.470 | 1.00 | 31.55 | 8 |
| | ATOM | 715 | N | GLY | A | 357 | 32.661 | 39.451 | 25.218 | 1.00 | 32.69 | 7 |
| | ATOM | 716 | CA | GLY | A | 357 | 32.511 | 38.304 | 24.338 | 1.00 | 29.87 | 6 |
| 55 | ATOM | 717 | C | GLY | A | 357 | 33.653 | 38.157 | 23.359 | 1.00 | 33.12 | 6 |
| | ATOM | 718 | O | GLY | A | 357 | 34.302 | 37.110 | 23.323 | 1.00 | 29.41 | 8 |
| | ATOM | 719 | N | MET | A | 358 | 33.876 | 39.206 | 22.564 | 1.00 | 33.31 | 7 |
| | ATOM | 720 | CA | MET | A | 358 | 34.949 | 39.206 | 21.580 | 1.00 | 35.87 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| 5 | ATOM | 721 | CB | MET | A | 358 | 35.143 | 40.606 | 21.009 | 1.00 | 34.56 | 6 |
| | ATOM | 722 | CG | MET | A | 358 | 33.949 | 41.145 | 20.290 | 1.00 | 46.43 | 6 |
| | ATOM | 723 | SD | MET | A | 358 | 34.207 | 42.776 | 19.514 | 1.00 | 42.13 | 16 |
| | ATOM | 724 | CE | MET | A | 358 | 34.507 | 43.855 | 20.994 | 1.00 | 44.29 | 6 |
| | ATOM | 725 | C | MET | A | 358 | 36.256 | 38.762 | 22.230 | 1.00 | 33.26 | 6 |
| 10 | ATOM | 726 | O | MET | A | 358 | 36.894 | 37.807 | 21.795 | 1.00 | 36.39 | 8 |
| | ATOM | 727 | N | SER | A | 359 | 36.637 | 39.491 | 23.281 | 1.00 | 33.31 | 7 |
| | ATOM | 728 | CA | SER | A | 359 | 37.860 | 39.226 | 24.019 | 1.00 | 34.39 | 6 |
| | ATOM | 729 | CB | SER | A | 359 | 37.869 | 40.067 | 25.295 | 1.00 | 30.84 | 6 |
| | ATOM | 730 | OG | SER | A | 359 | 39.135 | 40.008 | 25.930 | 1.00 | 47.14 | 8 |
| 15 | ATOM | 731 | C | SER | A | 359 | 37.984 | 37.748 | 24.357 | 1.00 | 36.43 | 6 |
| | ATOM | 732 | O | SER | A | 359 | 38.900 | 37.078 | 23.896 | 1.00 | 35.46 | 8 |
| | ATOM | 733 | N | LEU | A | 360 | 37.046 | 37.264 | 25.166 | 1.00 | 36.74 | 7 |
| | ATOM | 734 | CA | LEU | A | 360 | 37.017 | 35.875 | 25.604 | 1.00 | 35.44 | 6 |
| | ATOM | 735 | CB | LEU | A | 360 | 35.708 | 35.579 | 26.336 | 1.00 | 34.16 | 6 |
| 20 | ATOM | 736 | CG | LEU | A | 360 | 35.471 | 36.290 | 27.644 | 1.00 | 34.59 | 6 |
| | ATOM | 737 | CD1 | LEU | A | 360 | 34.225 | 35.765 | 28.312 | 1.00 | 33.53 | 6 |
| | ATOM | 738 | CD2 | LEU | A | 360 | 36.658 | 36.052 | 28.541 | 1.00 | 31.69 | 6 |
| | ATOM | 739 | C | LEU | A | 360 | 37.203 | 34.862 | 24.500 | 1.00 | 38.72 | 6 |
| | ATOM | 740 | O | LEU | A | 360 | 37.820 | 33.828 | 24.728 | 1.00 | 38.29 | 8 |
| 25 | ATOM | 741 | N | SER | A | 361 | 36.635 | 35.147 | 23.328 | 1.00 | 40.96 | 7 |
| | ATOM | 742 | CA | SER | A | 361 | 36.777 | 34.262 | 22.186 | 1.00 | 45.67 | 6 |
| | ATOM | 743 | CB | SER | A | 361 | 36.518 | 35.045 | 20.904 | 1.00 | 46.45 | 6 |
| | ATOM | 744 | OG | SER | A | 361 | 35.210 | 35.598 | 20.906 | 1.00 | 51.81 | 8 |
| | ATOM | 745 | C | SER | A | 361 | 38.166 | 33.627 | 22.145 | 1.00 | 44.49 | 6 |
| 30 | ATOM | 746 | O | SER | A | 361 | 38.347 | 32.538 | 21.625 | 1.00 | 46.67 | 8 |
| | ATOM | 747 | N | SER | A | 362 | 39.134 | 34.348 | 22.703 | 1.00 | 41.44 | 7 |
| | ATOM | 748 | CA | SER | A | 362 | 40.525 | 33.918 | 22.790 | 1.00 | 42.13 | 6 |
| | ATOM | 749 | CB | SER | A | 362 | 41.408 | 35.131 | 23.066 | 1.00 | 42.61 | 6 |
| | ATOM | 750 | OG | SER | A | 362 | 41.219 | 36.136 | 22.076 | 1.00 | 51.87 | 8 |
| 35 | ATOM | 751 | C | SER | A | 362 | 40.798 | 32.870 | 23.876 | 1.00 | 38.41 | 6 |
| | ATOM | 752 | O | SER | A | 362 | 41.553 | 31.938 | 23.641 | 1.00 | 38.01 | 8 |
| | ATOM | 753 | N | PHE | A | 363 | 40.198 | 33.039 | 25.058 | 1.00 | 34.55 | 7 |
| | ATOM | 754 | CA | PHE | A | 363 | 40.417 | 32.126 | 26.174 | 1.00 | 32.96 | 6 |
| | ATOM | 755 | CB | PHE | A | 363 | 39.832 | 32.718 | 27.447 | 1.00 | 31.99 | 6 |
| 40 | ATOM | 756 | CG | PHE | A | 363 | 40.448 | 34.036 | 27.840 | 1.00 | 29.97 | 6 |
| | ATOM | 757 | CD1 | PHE | A | 363 | 40.102 | 34.650 | 29.020 | 1.00 | 30.61 | 6 |
| | ATOM | 758 | CD2 | PHE | A | 363 | 41.379 | 34.646 | 27.014 | 1.00 | 32.02 | 6 |
| | ATOM | 759 | CE1 | PHE | A | 363 | 40.685 | 35.856 | 29.391 | 1.00 | 33.67 | 6 |
| | ATOM | 760 | CE2 | PHE | A | 363 | 41.959 | 35.843 | 27.377 | 1.00 | 30.91 | 6 |
| 45 | ATOM | 761 | CZ | PHE | A | 363 | 41.615 | 36.456 | 28.558 | 1.00 | 29.33 | 6 |
| | ATOM | 762 | C | PHE | A | 363 | 39.883 | 30.716 | 25.967 | 1.00 | 30.52 | 6 |
| | ATOM | 763 | O | PHE | A | 363 | 40.436 | 29.766 | 26.526 | 1.00 | 32.19 | 8 |
| | ATOM | 764 | N | ASN | A | 364 | 38.817 | 30.570 | 25.175 | 1.00 | 33.51 | 7 |
| | ATOM | 765 | CA | ASN | A | 364 | 38.239 | 29.264 | 24.918 | 1.00 | 38.03 | 6 |
| 50 | ATOM | 766 | CB | ASN | A | 364 | 39.240 | 28.404 | 24.139 | 1.00 | 42.32 | 6 |
| | ATOM | 767 | CG | ASN | A | 364 | 39.696 | 29.065 | 22.861 | 1.00 | 53.11 | 6 |
| | ATOM | 768 | OD1 | ASN | A | 364 | 38.874 | 29.330 | 21.954 | 1.00 | 59.51 | 8 |
| | ATOM | 769 | ND2 | ASN | A | 364 | 40.986 | 29.330 | 22.772 | 1.00 | 55.95 | 7 |
| | ATOM | 770 | C | ASN | A | 364 | 37.916 | 28.572 | 26.235 | 1.00 | 31.89 | 6 |
| 55 | ATOM | 771 | O | ASN | A | 364 | 38.324 | 27.428 | 26.457 | 1.00 | 30.28 | 8 |
| | ATOM | 772 | N | LEU | A | 365 | 37.176 | 29.271 | 27.094 | 1.00 | 27.62 | 7 |
| | ATOM | 773 | CA | LEU | A | 365 | 36.806 | 28.743 | 28.406 | 1.00 | 29.36 | 6 |
| | ATOM | 774 | CB | LEU | A | 365 | 36.195 | 29.866 | 29.237 | 1.00 | 27.54 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 775 | CG | LEU | A | 365 | 36.990 | 31.150 | 29.185 | 1.00 | 38.91 | 6 |
| | ATOM | 776 | CD1 | LEU | A | 365 | 36.316 | 32.216 | 30.036 | 1.00 | 34.47 | 6 |
| | ATOM | 777 | CD2 | LEU | A | 365 | 38.406 | 30.883 | 29.663 | 1.00 | 34.24 | 6 |
| | ATOM | 778 | C | LEU | A | 365 | 35.830 | 27.590 | 28.262 | 1.00 | 26.23 | 6 |
| | ATOM | 779 | O | LEU | A | 365 | 34.890 | 27.649 | 27.472 | 1.00 | 27.06 | 8 |
| 10 | ATOM | 780 | N | ASP | A | 366 | 36.083 | 26.528 | 29.021 | 1.00 | 25.23 | 7 |
| | ATOM | 781 | CA | ASP | A | 366 | 35.213 | 25.358 | 28.988 | 1.00 | 26.07 | 6 |
| | ATOM | 782 | CB | ASP | A | 366 | 36.027 | 24.049 | 29.033 | 1.00 | 29.68 | 6 |
| | ATOM | 783 | CG | ASP | A | 366 | 36.799 | 23.874 | 30.303 | 1.00 | 35.74 | 6 |
| | ATOM | 784 | OD1 | ASP | A | 366 | 36.285 | 24.177 | 31.402 | 1.00 | 36.78 | 8 |
| 15 | ATOM | 785 | OD2 | ASP | A | 366 | 37.959 | 23.386 | 30.240 | 1.00 | 41.23 | 8 |
| | ATOM | 786 | C | ASP | A | 366 | 34.278 | 25.434 | 30.181 | 1.00 | 27.70 | 6 |
| | ATOM | 787 | O | ASP | A | 366 | 34.587 | 26.097 | 31.173 | 1.00 | 31.94 | 8 |
| | ATOM | 788 | N | ASP | A | 367 | 33.141 | 24.743 | 30.066 | 1.00 | 29.18 | 7 |
| | ATOM | 789 | CA | ASP | A | 367 | 32.120 | 24.679 | 31.120 | 1.00 | 32.72 | 6 |
| 20 | ATOM | 790 | CB | ASP | A | 367 | 31.472 | 23.284 | 31.147 | 1.00 | 38.04 | 6 |
| | ATOM | 791 | CG | ASP | A | 367 | 30.806 | 22.924 | 29.854 | 1.00 | 42.43 | 6 |
| | ATOM | 792 | OD1 | ASP | A | 367 | 29.877 | 23.650 | 29.409 | 1.00 | 35.95 | 8 |
| | ATOM | 793 | OD2 | ASP | A | 367 | 31.186 | 21.884 | 29.250 | 1.00 | 51.42 | 8 |
| | ATOM | 794 | C | ASP | A | 367 | 32.754 | 24.969 | 32.482 | 1.00 | 33.71 | 6 |
| 25 | ATOM | 795 | O | ASP | A | 367 | 32.484 | 26.000 | 33.098 | 1.00 | 38.30 | 8 |
| | ATOM | 796 | N | THR | A | 368 | 33.602 | 24.032 | 32.919 | 1.00 | 31.06 | 7 |
| | ATOM | 797 | CA | THR | A | 368 | 34.329 | 24.124 | 34.181 | 1.00 | 26.28 | 6 |
| | ATOM | 798 | CB | THR | A | 368 | 35.559 | 23.222 | 34.141 | 1.00 | 27.30 | 6 |
| | ATOM | 799 | OG1 | THR | A | 368 | 35.161 | 21.871 | 33.885 | 1.00 | 33.42 | 8 |
| 30 | ATOM | 800 | CG2 | THR | A | 368 | 36.323 | 23.303 | 35.454 | 1.00 | 25.16 | 6 |
| | ATOM | 801 | C | THR | A | 368 | 34.764 | 25.557 | 34.479 | 1.00 | 21.13 | 6 |
| | ATOM | 802 | O | THR | A | 368 | 34.408 | 26.153 | 35.503 | 1.00 | 23.17 | 8 |
| | ATOM | 803 | N | GLU | A | 369 | 35.545 | 26.092 | 33.551 | 1.00 | 21.32 | 7 |
| | ATOM | 804 | CA | GLU | A | 369 | 36.065 | 27.435 | 33.661 | 1.00 | 28.00 | 6 |
| 35 | ATOM | 805 | CB | GLU | A | 369 | 36.960 | 27.707 | 32.453 | 1.00 | 32.79 | 6 |
| | ATOM | 806 | CG | GLU | A | 369 | 38.089 | 26.663 | 32.346 | 1.00 | 36.29 | 6 |
| | ATOM | 807 | CD | GLU | A | 369 | 38.906 | 26.747 | 31.110 | 1.00 | 41.03 | 6 |
| | ATOM | 808 | OE1 | GLU | A | 369 | 38.337 | 26.744 | 29.994 | 1.00 | 42.05 | 8 |
| | ATOM | 809 | OE2 | GLU | A | 369 | 40.158 | 26.795 | 31.218 | 1.00 | 42.03 | 8 |
| 40 | ATOM | 810 | C | GLU | A | 369 | 34.953 | 28.471 | 33.821 | 1.00 | 25.57 | 6 |
| | ATOM | 811 | O | GLU | A | 369 | 34.987 | 29.256 | 34.760 | 1.00 | 20.56 | 8 |
| | ATOM | 812 | N | VAL | A | 370 | 33.967 | 28.463 | 32.921 | 1.00 | 25.39 | 7 |
| | ATOM | 813 | CA | VAL | A | 370 | 32.849 | 29.396 | 33.029 | 1.00 | 25.99 | 6 |
| | ATOM | 814 | CB | VAL | A | 370 | 31.763 | 29.131 | 31.987 | 1.00 | 26.15 | 6 |
| 45 | ATOM | 815 | CG1 | VAL | A | 370 | 30.609 | 30.093 | 32.183 | 1.00 | 27.65 | 6 |
| | ATOM | 816 | CG2 | VAL | A | 370 | 32.306 | 29.251 | 30.592 | 1.00 | 17.70 | 6 |
| | ATOM | 817 | C | VAL | A | 370 | 32.245 | 29.209 | 34.412 | 1.00 | 26.49 | 6 |
| | ATOM | 818 | O | VAL | A | 370 | 32.012 | 30.170 | 35.147 | 1.00 | 28.16 | 8 |
| | ATOM | 819 | N | ALA | A | 371 | 31.988 | 27.947 | 34.739 | 1.00 | 21.01 | 7 |
| 50 | ATOM | 820 | CA | ALA | A | 371 | 31.393 | 27.554 | 36.011 | 1.00 | 19.57 | 6 |
| | ATOM | 821 | CB | ALA | A | 371 | 31.441 | 26.039 | 36.145 | 1.00 | 18.62 | 6 |
| | ATOM | 822 | C | ALA | A | 371 | 32.116 | 28.211 | 37.177 | 1.00 | 23.48 | 6 |
| | ATOM | 823 | O | ALA | A | 371 | 31.531 | 28.989 | 37.931 | 1.00 | 32.67 | 8 |
| | ATOM | 824 | N | LEU | A | 372 | 33.401 | 27.893 | 37.305 | 1.00 | 22.89 | 7 |
| 55 | ATOM | 825 | CA | LEU | A | 372 | 34.217 | 28.447 | 38.369 | 1.00 | 23.28 | 6 |
| | ATOM | 826 | CB | LEU | A | 372 | 35.675 | 27.996 | 38.178 | 1.00 | 27.76 | 6 |
| | ATOM | 827 | CG | LEU | A | 372 | 35.943 | 26.524 | 38.415 | 1.00 | 21.18 | 6 |
| | ATOM | 828 | CD1 | LEU | A | 372 | 37.356 | 26.171 | 38.049 | 1.00 | 27.64 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| 5 | ATOM | 829 | CD2 | LEU | A | 372 | 35.675 | 26.204 | 39.880 | 1.00 | 20.90 | 6 |
| | ATOM | 830 | C | LEU | A | 372 | 34.098 | 29.966 | 38.396 | 1.00 | 21.34 | 6 |
| | ATOM | 831 | O | LEU | A | 372 | 33.828 | 30.572 | 39.439 | 1.00 | 23.16 | 8 |
| | ATOM | 832 | N | LEU | A | 373 | 34.288 | 30.561 | 37.223 | 1.00 | 24.42 | 7 |
| | ATOM | 833 | CA | LEU | A | 373 | 34.214 | 32.007 | 37.074 | 1.00 | 23.78 | 6 |
| 10 | ATOM | 834 | CB | LEU | A | 373 | 34.296 | 32.360 | 35.575 | 1.00 | 22.18 | 6 |
| | ATOM | 835 | CG | LEU | A | 373 | 34.784 | 33.726 | 35.165 | 1.00 | 31.52 | 6 |
| | ATOM | 836 | CD1 | LEU | A | 373 | 36.000 | 34.084 | 35.962 | 1.00 | 31.93 | 6 |
| | ATOM | 837 | CD2 | LEU | A | 373 | 35.103 | 33.720 | 33.693 | 1.00 | 30.24 | 6 |
| | ATOM | 838 | C | LEU | A | 373 | 32.904 | 32.480 | 37.720 | 1.00 | 25.69 | 6 |
| 15 | ATOM | 839 | O | LEU | A | 373 | 32.895 | 33.410 | 38.532 | 1.00 | 30.13 | 8 |
| | ATOM | 840 | N | GLN | A | 374 | 31.814 | 31.800 | 37.368 | 1.00 | 26.24 | 7 |
| | ATOM | 841 | CA | GLN | A | 374 | 30.487 | 32.104 | 37.896 | 1.00 | 21.60 | 6 |
| | ATOM | 842 | CB | GLN | A | 374 | 29.454 | 31.121 | 37.335 | 1.00 | 24.57 | 6 |
| | ATOM | 843 | CG | GLN | A | 374 | 29.310 | 31.145 | 35.821 | 1.00 | 21.02 | 6 |
| 20 | ATOM | 844 | CD | GLN | A | 374 | 28.224 | 30.201 | 35.331 | 1.00 | 22.86 | 6 |
| | ATOM | 845 | OE1 | GLN | A | 374 | 28.037 | 30.042 | 34.123 | 1.00 | 24.07 | 8 |
| | ATOM | 846 | NE2 | GLN | A | 374 | 27.515 | 29.590 | 36.249 | 1.00 | 25.59 | 7 |
| | ATOM | 847 | C | GLN | A | 374 | 30.421 | 32.039 | 39.422 | 1.00 | 20.66 | 6 |
| | ATOM | 848 | O | GLN | A | 374 | 29.717 | 32.832 | 40.048 | 1.00 | 24.47 | 8 |
| 25 | ATOM | 849 | N | ALA | A | 375 | 31.136 | 31.074 | 40.004 | 1.00 | 16.26 | 7 |
| | ATOM | 850 | CA | ALA | A | 375 | 31.155 | 30.889 | 41.445 | 1.00 | 17.16 | 6 |
| | ATOM | 851 | CB | ALA | A | 375 | 31.805 | 29.568 | 41.780 | 1.00 | 19.53 | 6 |
| | ATOM | 852 | C | ALA | A | 375 | 31.907 | 32.025 | 42.108 | 1.00 | 25.13 | 6 |
| | ATOM | 853 | O | ALA | A | 375 | 31.397 | 32.646 | 43.034 | 1.00 | 23.81 | 8 |
| 30 | ATOM | 854 | N | VAL | A | 376 | 33.122 | 32.277 | 41.611 | 1.00 | 24.57 | 7 |
| | ATOM | 855 | CA | VAL | A | 376 | 33.959 | 33.354 | 42.118 | 1.00 | 25.80 | 6 |
| | ATOM | 856 | CB | VAL | A | 376 | 35.101 | 33.658 | 41.164 | 1.00 | 26.48 | 6 |
| | ATOM | 857 | CG1 | VAL | A | 376 | 35.926 | 34.812 | 41.697 | 1.00 | 23.20 | 6 |
| | ATOM | 858 | CG2 | VAL | A | 376 | 35.959 | 32.429 | 40.952 | 1.00 | 19.08 | 6 |
| 35 | ATOM | 859 | C | VAL | A | 376 | 33.107 | 34.599 | 42.312 | 1.00 | 25.69 | 6 |
| | ATOM | 860 | O | VAL | A | 376 | 33.297 | 35.364 | 43.251 | 1.00 | 27.87 | 8 |
| | ATOM | 861 | N | LEU | A | 377 | 32.159 | 34.781 | 41.399 | 1.00 | 23.09 | 7 |
| | ATOM | 862 | CA | LEU | A | 377 | 31.242 | 35.915 | 41.423 | 1.00 | 22.86 | 6 |
| | ATOM | 863 | CB | LEU | A | 377 | 30.540 | 36.031 | 40.061 | 1.00 | 18.50 | 6 |
| 40 | ATOM | 864 | CG | LEU | A | 377 | 31.424 | 36.368 | 38.885 | 1.00 | 22.65 | 6 |
| | ATOM | 865 | CD1 | LEU | A | 377 | 30.689 | 36.227 | 37.601 | 1.00 | 16.70 | 6 |
| | ATOM | 866 | CD2 | LEU | A | 377 | 31.916 | 37.776 | 39.051 | 1.00 | 19.58 | 6 |
| | ATOM | 867 | C | LEU | A | 377 | 30.228 | 35.719 | 42.543 | 1.00 | 26.14 | 6 |
| | ATOM | 868 | O | LEU | A | 377 | 30.131 | 36.532 | 43.452 | 1.00 | 20.62 | 8 |
| 45 | ATOM | 869 | N | LEU | A | 378 | 29.483 | 34.614 | 42.468 | 1.00 | 28.99 | 7 |
| | ATOM | 870 | CA | LEU | A | 378 | 28.469 | 34.303 | 43.475 | 1.00 | 28.87 | 6 |
| | ATOM | 871 | CB | LEU | A | 378 | 28.053 | 32.826 | 43.397 | 1.00 | 26.89 | 6 |
| | ATOM | 872 | CG | LEU | A | 378 | 27.110 | 32.344 | 44.472 | 1.00 | 28.83 | 6 |
| | ATOM | 873 | CD1 | LEU | A | 378 | 25.915 | 33.252 | 44.525 | 1.00 | 27.97 | 6 |
| 50 | ATOM | 874 | CD2 | LEU | A | 378 | 26.693 | 30.928 | 44.205 | 1.00 | 27.69 | 6 |
| | ATOM | 875 | C | LEU | A | 378 | 28.992 | 34.617 | 44.853 | 1.00 | 31.09 | 6 |
| | ATOM | 876 | O | LEU | A | 378 | 28.399 | 35.421 | 45.573 | 1.00 | 31.77 | 8 |
| | ATOM | 877 | N | MET | A | 379 | 30.118 | 33.991 | 45.189 | 1.00 | 31.44 | 7 |
| | ATOM | 878 | CA | MET | A | 379 | 30.736 | 34.141 | 46.494 | 1.00 | 32.62 | 6 |
| 55 | ATOM | 879 | CB | MET | A | 379 | 31.690 | 32.960 | 46.744 | 1.00 | 31.45 | 6 |
| | ATOM | 880 | CG | MET | A | 379 | 30.984 | 31.595 | 46.792 | 1.00 | 38.75 | 6 |
| | ATOM | 881 | SD | MET | A | 379 | 29.741 | 31.626 | 48.107 | 1.00 | 41.27 | 16 |
| | ATOM | 882 | CE | MET | A | 379 | 28.896 | 30.036 | 47.851 | 1.00 | 35.68 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 883 | C | MET | A | 379 | 31.485 | 35.448 | 46.727 | 1.00 | 33.72 | 6 |
| | ATOM | 884 | O | MET | A | 379 | 32.567 | 35.450 | 47.305 | 1.00 | 36.29 | 8 |
| | ATOM | 885 | N | SER | A | 380 | 30.889 | 36.555 | 46.315 | 1.00 | 34.49 | 7 |
| | ATOM | 886 | CA | SER | A | 380 | 31.498 | 37.853 | 46.550 | 1.00 | 33.97 | 6 |
| | ATOM | 887 | CB | SER | A | 380 | 30.921 | 38.890 | 45.576 | 1.00 | 31.24 | 6 |
| 10 | ATOM | 888 | OG | SER | A | 380 | 31.205 | 38.543 | 44.230 | 1.00 | 39.42 | 8 |
| | ATOM | 889 | C | SER | A | 380 | 31.179 | 38.239 | 47.992 | 1.00 | 39.69 | 6 |
| | ATOM | 890 | O | SER | A | 380 | 30.029 | 38.446 | 48.357 | 1.00 | 44.64 | 8 |
| | ATOM | 891 | N | SER | A | 381 | 32.214 | 38.313 | 48.812 | 1.00 | 41.04 | 7 |
| | ATOM | 892 | CA | SER | A | 381 | 32.060 | 38.640 | 50.216 | 1.00 | 44.91 | 6 |
| 15 | ATOM | 893 | CB | SER | A | 381 | 33.324 | 38.234 | 50.951 | 1.00 | 44.50 | 6 |
| | ATOM | 894 | OG | SER | A | 381 | 34.431 | 39.002 | 50.510 | 1.00 | 45.42 | 8 |
| | ATOM | 895 | C | SER | A | 381 | 31.795 | 40.106 | 50.499 | 1.00 | 44.59 | 6 |
| | ATOM | 896 | O | SER | A | 381 | 31.476 | 40.470 | 51.618 | 1.00 | 49.32 | 8 |
| | ATOM | 897 | N | ASP | A | 382 | 31.939 | 40.942 | 49.486 | 1.00 | 43.75 | 7 |
| 20 | ATOM | 898 | CA | ASP | A | 382 | 31.744 | 42.362 | 49.641 | 1.00 | 43.93 | 6 |
| | ATOM | 899 | CB | ASP | A | 382 | 32.673 | 43.111 | 48.677 | 1.00 | 48.39 | 6 |
| | ATOM | 900 | CG | ASP | A | 382 | 32.572 | 42.624 | 47.263 | 1.00 | 53.23 | 6 |
| | ATOM | 901 | OD1 | ASP | A | 382 | 32.705 | 41.400 | 47.034 | 1.00 | 56.97 | 8 |
| | ATOM | 902 | OD2 | ASP | A | 382 | 32.358 | 43.454 | 46.333 | 1.00 | 58.91 | 8 |
| 25 | ATOM | 903 | C | ASP | A | 382 | 30.314 | 42.885 | 49.507 | 1.00 | 41.09 | 6 |
| | ATOM | 904 | O | ASP | A | 382 | 30.048 | 44.036 | 49.845 | 1.00 | 40.93 | 8 |
| | ATOM | 905 | N | ARG | A | 383 | 29.397 | 42.049 | 49.034 | 1.00 | 42.63 | 7 |
| | ATOM | 906 | CA | ARG | A | 383 | 28.036 | 42.485 | 48.876 | 1.00 | 43.32 | 6 |
| | ATOM | 907 | CB | ARG | A | 383 | 27.138 | 41.332 | 48.443 | 1.00 | 42.31 | 6 |
| 30 | ATOM | 908 | CG | ARG | A | 383 | 27.651 | 40.399 | 47.352 | 1.00 | 40.83 | 6 |
| | ATOM | 909 | CD | ARG | A | 383 | 27.586 | 40.954 | 45.925 | 1.00 | 38.09 | 6 |
| | ATOM | 910 | NE | ARG | A | 383 | 27.768 | 39.878 | 44.975 | 1.00 | 37.33 | 7 |
| | ATOM | 911 | CZ | ARG | A | 383 | 28.037 | 40.058 | 43.693 | 1.00 | 38.35 | 6 |
| | ATOM | 912 | NH1 | ARG | A | 383 | 28.142 | 41.292 | 43.198 | 1.00 | 33.70 | 7 |
| 35 | ATOM | 913 | NH2 | ARG | A | 383 | 28.194 | 38.992 | 42.918 | 1.00 | 35.46 | 7 |
| | ATOM | 914 | C | ARG | A | 383 | 27.523 | 42.989 | 50.216 | 1.00 | 44.96 | 6 |
| | ATOM | 915 | O | ARG | A | 383 | 27.744 | 42.344 | 51.260 | 1.00 | 45.60 | 8 |
| | ATOM | 916 | N | PRO | A | 384 | 26.852 | 44.144 | 50.223 | 1.00 | 45.33 | 7 |
| | ATOM | 917 | CD | PRO | A | 384 | 26.625 | 44.964 | 49.027 | 1.00 | 46.85 | 6 |
| 40 | ATOM | 918 | CA | PRO | A | 384 | 26.298 | 44.738 | 51.446 | 1.00 | 47.37 | 6 |
| | ATOM | 919 | CB | PRO | A | 384 | 25.841 | 46.130 | 51.012 | 1.00 | 46.90 | 6 |
| | ATOM | 920 | CG | PRO | A | 384 | 26.075 | 46.229 | 49.567 | 1.00 | 46.41 | 6 |
| | ATOM | 921 | C | PRO | A | 384 | 25.158 | 43.919 | 52.049 | 1.00 | 48.29 | 6 |
| | ATOM | 922 | O | PRO | A | 384 | 24.404 | 43.264 | 51.329 | 1.00 | 48.34 | 8 |
| 45 | ATOM | 923 | N | GLY | A | 385 | 25.039 | 43.983 | 53.383 | 1.00 | 49.88 | 7 |
| | ATOM | 924 | CA | GLY | A | 385 | 23.991 | 43.270 | 54.113 | 1.00 | 50.35 | 6 |
| | ATOM | 925 | C | GLY | A | 385 | 24.347 | 41.852 | 54.495 | 1.00 | 50.70 | 6 |
| | ATOM | 926 | O | GLY | A | 385 | 23.614 | 41.204 | 55.244 | 1.00 | 53.48 | 8 |
| | ATOM | 927 | N | LEU | A | 386 | 25.466 | 41.371 | 53.955 | 1.00 | 49.04 | 7 |
| 50 | ATOM | 928 | CA | LEU | A | 386 | 25.901 | 40.017 | 54.215 | 1.00 | 50.53 | 6 |
| | ATOM | 929 | CB | LEU | A | 386 | 27.224 | 39.751 | 53.492 | 1.00 | 45.17 | 6 |
| | ATOM | 930 | CG | LEU | A | 386 | 27.152 | 39.592 | 51.993 | 1.00 | 48.26 | 6 |
| | ATOM | 931 | CD1 | LEU | A | 386 | 28.542 | 39.439 | 51.404 | 1.00 | 41.68 | 6 |
| | ATOM | 932 | CD2 | LEU | A | 386 | 26.302 | 38.374 | 51.682 | 1.00 | 38.40 | 6 |
| 55 | ATOM | 933 | C | LEU | A | 386 | 26.045 | 39.776 | 55.691 | 1.00 | 52.13 | 6 |
| | ATOM | 934 | O | LEU | A | 386 | 26.296 | 40.692 | 56.459 | 1.00 | 53.67 | 8 |
| | ATOM | 935 | N | ALA | A | 387 | 25.861 | 38.522 | 56.077 | 1.00 | 53.42 | 7 |
| | ATOM | 936 | CA | ALA | A | 387 | 25.976 | 38.129 | 57.470 | 1.00 | 56.01 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| 5 | ATOM | 937 | CB | ALA | A | 387 | 24.802 | 37.234 | 57.854 | 1.00 | 56.47 | 6 |
| | ATOM | 938 | C | ALA | A | 387 | 27.289 | 37.385 | 57.659 | 1.00 | 55.52 | 6 |
| | ATOM | 939 | O | ALA | A | 387 | 28.275 | 37.940 | 58.134 | 1.00 | 53.75 | 8 |
| | ATOM | 940 | N | CYS | A | 388 | 27.273 | 36.120 | 57.253 | 1.00 | 56.03 | 7 |
| | ATOM | 941 | CA | CYS | A | 388 | 28.412 | 35.236 | 57.370 | 1.00 | 59.57 | 6 |
| 10 | ATOM | 942 | CB | CYS | A | 388 | 27.923 | 33.803 | 57.172 | 1.00 | 59.23 | 6 |
| | ATOM | 943 | SG | CYS | A | 388 | 26.397 | 33.431 | 58.009 | 1.00 | 58.64 | 16 |
| | ATOM | 944 | C | CYS | A | 388 | 29.482 | 35.581 | 56.328 | 1.00 | 62.18 | 6 |
| | ATOM | 945 | O | CYS | A | 388 | 29.720 | 34.821 | 55.400 | 1.00 | 67.88 | 8 |
| | ATOM | 946 | N | VAL | A | 389 | 30.110 | 36.747 | 56.495 | 1.00 | 60.78 | 7 |
| 15 | ATOM | 947 | CA | VAL | A | 389 | 31.173 | 37.212 | 55.590 | 1.00 | 57.70 | 6 |
| | ATOM | 948 | CB | VAL | A | 389 | 31.740 | 38.567 | 56.024 | 1.00 | 57.09 | 6 |
| | ATOM | 949 | CG1 | VAL | A | 389 | 32.795 | 39.037 | 55.041 | 1.00 | 59.03 | 6 |
| | ATOM | 950 | CG2 | VAL | A | 389 | 30.640 | 39.598 | 56.171 | 1.00 | 53.98 | 6 |
| | ATOM | 951 | C | VAL | A | 389 | 32.297 | 36.182 | 55.550 | 1.00 | 57.77 | 6 |
| 20 | ATOM | 952 | O | VAL | A | 389 | 32.358 | 35.336 | 54.662 | 1.00 | 60.94 | 8 |
| | ATOM | 953 | N | ALA | A | 390 | 33.182 | 36.292 | 56.528 | 1.00 | 52.68 | 7 |
| | ATOM | 954 | CA | ALA | A | 390 | 34.347 | 35.431 | 56.684 | 1.00 | 48.41 | 6 |
| | ATOM | 955 | CB | ALA | A | 390 | 34.703 | 35.321 | 58.185 | 1.00 | 45.19 | 6 |
| | ATOM | 956 | C | ALA | A | 390 | 34.224 | 34.040 | 56.082 | 1.00 | 47.63 | 6 |
| 25 | ATOM | 957 | O | ALA | A | 390 | 35.107 | 33.597 | 55.348 | 1.00 | 51.95 | 8 |
| | ATOM | 958 | N | ARG | A | 391 | 33.117 | 33.366 | 56.391 | 1.00 | 47.11 | 7 |
| | ATOM | 959 | CA | ARG | A | 391 | 32.879 | 32.018 | 55.885 | 1.00 | 51.64 | 6 |
| | ATOM | 960 | CB | ARG | A | 391 | 31.520 | 31.498 | 56.383 | 1.00 | 54.22 | 6 |
| | ATOM | 961 | CG | ARG | A | 391 | 31.267 | 30.012 | 56.059 | 1.00 | 64.20 | 6 |
| 30 | ATOM | 962 | CD | ARG | A | 391 | 29.930 | 29.489 | 56.602 | 1.00 | 73.80 | 6 |
| | ATOM | 963 | NE | ARG | A | 391 | 29.787 | 28.044 | 56.454 | 1.00 | 79.76 | 7 |
| | ATOM | 964 | CZ | ARG | A | 391 | 30.573 | 27.140 | 57.043 | 1.00 | 84.27 | 6 |
| | ATOM | 965 | NH1 | ARG | A | 391 | 31.598 | 27.535 | 57.806 | 1.00 | 85.28 | 7 |
| | ATOM | 966 | NH2 | ARG | A | 391 | 30.340 | 25.840 | 56.849 | 1.00 | 86.84 | 7 |
| 35 | ATOM | 967 | C | ARG | A | 391 | 32.922 | 31.986 | 54.358 | 1.00 | 48.18 | 6 |
| | ATOM | 968 | O | ARG | A | 391 | 33.494 | 31.080 | 53.756 | 1.00 | 49.57 | 8 |
| | ATOM | 969 | N | ILE | A | 392 | 32.281 | 32.993 | 53.762 | 1.00 | 45.01 | 7 |
| | ATOM | 970 | CA | ILE | A | 392 | 32.196 | 33.148 | 52.319 | 1.00 | 48.77 | 6 |
| | ATOM | 971 | CB | ILE | A | 392 | 31.224 | 34.297 | 51.963 | 1.00 | 46.45 | 6 |
| 40 | ATOM | 972 | CG2 | ILE | A | 392 | 31.241 | 34.582 | 50.479 | 1.00 | 42.35 | 6 |
| | ATOM | 973 | CG1 | ILE | A | 392 | 29.791 | 33.953 | 52.402 | 1.00 | 49.69 | 6 |
| | ATOM | 974 | CD1 | ILE | A | 392 | 28.792 | 35.039 | 52.113 | 1.00 | 51.09 | 6 |
| | ATOM | 975 | C | ILE | A | 392 | 33.554 | 33.356 | 51.641 | 1.00 | 50.90 | 6 |
| | ATOM | 976 | O | ILE | A | 392 | 33.914 | 32.605 | 50.732 | 1.00 | 52.21 | 8 |
| 45 | ATOM | 977 | N | GLU | A | 393 | 34.298 | 34.374 | 52.071 | 1.00 | 50.43 | 7 |
| | ATOM | 978 | CA | GLU | A | 393 | 35.592 | 34.684 | 51.471 | 1.00 | 50.30 | 6 |
| | ATOM | 979 | CB | GLU | A | 393 | 36.437 | 35.561 | 52.387 | 1.00 | 53.97 | 6 |
| | ATOM | 980 | CG | GLU | A | 393 | 36.558 | 36.966 | 51.844 | 1.00 | 62.18 | 6 |
| | ATOM | 981 | CD | GLU | A | 393 | 37.546 | 37.777 | 52.564 | 1.00 | 67.69 | 6 |
| 50 | ATOM | 982 | OE1 | GLU | A | 393 | 38.149 | 38.741 | 52.119 | 1.00 | 66.42 | 8 |
| | ATOM | 983 | OE2 | GLU | A | 393 | 37.856 | 37.640 | 53.729 | 1.00 | 70.64 | 8 |
| | ATOM | 984 | C | GLU | A | 393 | 36.341 | 33.429 | 51.230 | 1.00 | 49.31 | 6 |
| | ATOM | 985 | O | GLU | A | 393 | 36.755 | 33.089 | 50.125 | 1.00 | 49.53 | 8 |
| | ATOM | 986 | N | LYS | A | 394 | 36.552 | 32.730 | 52.303 | 1.00 | 46.07 | 7 |
| 55 | ATOM | 987 | CA | LYS | A | 394 | 37.265 | 31.543 | 52.078 | 1.00 | 45.76 | 6 |
| | ATOM | 988 | CB | LYS | A | 394 | 37.396 | 30.800 | 53.373 | 1.00 | 43.85 | 6 |
| | ATOM | 989 | CG | LYS | A | 394 | 38.207 | 31.617 | 54.394 | 1.00 | 40.00 | 6 |
| | ATOM | 990 | CD | LYS | A | 394 | 39.372 | 32.374 | 53.705 | 1.00 | 40.00 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 991 | CE | LYS | A | 394 | 40.136 | 33.265 | 54.681 | 1.00 | 40.00 | 6 |
| | ATOM | 992 | NZ | LYS | A | 394 | 41.516 | 33.602 | 54.162 | 1.00 | 40.00 | 7 |
| | ATOM | 993 | C | LYS | A | 394 | 36.568 | 30.778 | 50.966 | 1.00 | 46.69 | 6 |
| | ATOM | 994 | O | LYS | A | 394 | 37.215 | 30.427 | 49.988 | 1.00 | 49.13 | 8 |
| | ATOM | 995 | N | TYR | A | 395 | 35.269 | 30.514 | 51.095 | 1.00 | 46.57 | 7 |
| 10 | ATOM | 996 | CA | TYR | A | 395 | 34.553 | 29.823 | 50.022 | 1.00 | 43.33 | 6 |
| | ATOM | 997 | CB | TYR | A | 395 | 33.059 | 30.123 | 50.076 | 1.00 | 48.44 | 6 |
| | ATOM | 998 | CG | TYR | A | 395 | 32.275 | 29.236 | 50.994 | 1.00 | 53.83 | 6 |
| | ATOM | 999 | CD1 | TYR | A | 395 | 31.010 | 29.598 | 51.415 | 1.00 | 56.43 | 6 |
| | ATOM | 1000 | CE1 | TYR | A | 395 | 30.266 | 28.769 | 52.252 | 1.00 | 59.73 | 6 |
| 15 | ATOM | 1001 | CD2 | TYR | A | 395 | 32.790 | 28.033 | 51.428 | 1.00 | 56.47 | 6 |
| | ATOM | 1002 | CE2 | TYR | A | 395 | 32.054 | 27.198 | 52.265 | 1.00 | 62.60 | 6 |
| | ATOM | 1003 | CZ | TYR | A | 395 | 30.787 | 27.565 | 52.687 | 1.00 | 63.18 | 6 |
| | ATOM | 1004 | OH | TYR | A | 395 | 30.059 | 26.753 | 53.528 | 1.00 | 64.46 | 8 |
| | ATOM | 1005 | C | TYR | A | 395 | 35.120 | 30.356 | 48.716 | 1.00 | 37.30 | 6 |
| 20 | ATOM | 1006 | O | TYR | A | 395 | 35.643 | 29.601 | 47.908 | 1.00 | 34.10 | 8 |
| | ATOM | 1007 | N | GLN | A | 396 | 35.029 | 31.670 | 48.522 | 1.00 | 31.92 | 7 |
| | ATOM | 1008 | CA | GLN | A | 396 | 35.563 | 32.273 | 47.305 | 1.00 | 34.81 | 6 |
| | ATOM | 1009 | CB | GLN | A | 396 | 35.403 | 33.801 | 47.329 | 1.00 | 32.64 | 6 |
| | ATOM | 1010 | CG | GLN | A | 396 | 36.088 | 34.485 | 46.162 | 1.00 | 29.57 | 6 |
| 25 | ATOM | 1011 | CD | GLN | A | 396 | 35.616 | 35.891 | 45.927 | 1.00 | 29.46 | 6 |
| | ATOM | 1012 | OE1 | GLN | A | 396 | 35.599 | 36.726 | 46.862 | 1.00 | 34.65 | 8 |
| | ATOM | 1013 | NE2 | GLN | A | 396 | 35.245 | 36.173 | 44.689 | 1.00 | 27.21 | 7 |
| | ATOM | 1014 | C | GLN | A | 396 | 37.035 | 31.909 | 47.167 | 1.00 | 37.13 | 6 |
| | ATOM | 1015 | O | GLN | A | 396 | 37.511 | 31.590 | 46.080 | 1.00 | 37.36 | 8 |
| 30 | ATOM | 1016 | N | ASP | A | 397 | 37.751 | 31.970 | 48.285 | 1.00 | 38.61 | 7 |
| | ATOM | 1017 | CA | ASP | A | 397 | 39.164 | 31.642 | 48.298 | 1.00 | 40.37 | 6 |
| | ATOM | 1018 | CB | ASP | A | 397 | 39.757 | 31.869 | 49.704 | 1.00 | 40.51 | 6 |
| | ATOM | 1019 | CG | ASP | A | 397 | 39.813 | 33.319 | 50.095 | 1.00 | 43.77 | 6 |
| | ATOM | 1020 | OD1 | ASP | A | 397 | 40.397 | 34.123 | 49.334 | 1.00 | 46.50 | 8 |
| 35 | ATOM | 1021 | OD2 | ASP | A | 397 | 39.299 | 33.702 | 51.184 | 1.00 | 51.34 | 8 |
| | ATOM | 1022 | C | ASP | A | 397 | 39.302 | 30.176 | 47.898 | 1.00 | 38.62 | 6 |
| | ATOM | 1023 | O | ASP | A | 397 | 40.230 | 29.809 | 47.199 | 1.00 | 39.20 | 8 |
| | ATOM | 1024 | N | SER | A | 398 | 38.350 | 29.359 | 48.344 | 1.00 | 37.84 | 7 |
| | ATOM | 1025 | CA | SER | A | 398 | 38.348 | 27.929 | 48.063 | 1.00 | 37.80 | 6 |
| 40 | ATOM | 1026 | CB | SER | A | 398 | 37.240 | 27.240 | 48.878 | 1.00 | 34.28 | 6 |
| | ATOM | 1027 | OG | SER | A | 398 | 37.297 | 25.826 | 48.755 | 1.00 | 46.60 | 8 |
| | ATOM | 1028 | C | SER | A | 398 | 38.164 | 27.639 | 46.581 | 1.00 | 38.41 | 6 |
| | ATOM | 1029 | O | SER | A | 398 | 38.677 | 26.642 | 46.075 | 1.00 | 39.98 | 8 |
| | ATOM | 1030 | N | PHE | A | 399 | 37.419 | 28.507 | 45.893 | 1.00 | 34.82 | 7 |
| 45 | ATOM | 1031 | CA | PHE | A | 399 | 37.181 | 28.325 | 44.462 | 1.00 | 35.96 | 6 |
| | ATOM | 1032 | CB | PHE | A | 399 | 35.873 | 28.983 | 44.015 | 1.00 | 35.75 | 6 |
| | ATOM | 1033 | CG | PHE | A | 399 | 34.632 | 28.216 | 44.403 | 1.00 | 39.30 | 6 |
| | ATOM | 1034 | CD1 | PHE | A | 399 | 34.107 | 28.294 | 45.677 | 1.00 | 39.86 | 6 |
| | ATOM | 1035 | CD2 | PHE | A | 399 | 34.018 | 27.393 | 43.488 | 1.00 | 36.81 | 6 |
| 50 | ATOM | 1036 | CE1 | PHE | A | 399 | 32.961 | 27.557 | 46.013 | 1.00 | 41.25 | 6 |
| | ATOM | 1037 | CE2 | PHE | A | 399 | 32.880 | 26.661 | 43.825 | 1.00 | 43.61 | 6 |
| | ATOM | 1038 | CZ | PHE | A | 399 | 32.354 | 26.740 | 45.087 | 1.00 | 40.34 | 6 |
| | ATOM | 1039 | C | PHE | A | 399 | 38.328 | 28.890 | 43.630 | 1.00 | 33.48 | 6 |
| | ATOM | 1040 | O | PHE | A | 399 | 38.867 | 28.200 | 42.756 | 1.00 | 26.86 | 8 |
| 55 | ATOM | 1041 | N | LEU | A | 400 | 38.680 | 30.156 | 43.877 | 1.00 | 31.47 | 7 |
| | ATOM | 1042 | CA | LEU | A | 400 | 39.754 | 30.796 | 43.132 | 1.00 | 37.41 | 6 |
| | ATOM | 1043 | CB | LEU | A | 400 | 40.179 | 32.100 | 43.814 | 1.00 | 34.24 | 6 |
| | ATOM | 1044 | CG | LEU | A | 400 | 39.239 | 33.265 | 43.628 | 1.00 | 35.10 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 1045 | CD1 | LEU | A | 400 | 39.803 | 34.531 | 44.256 | 1.00 | 26.60 | 6 |
| | ATOM | 1046 | CD2 | LEU | A | 400 | 39.065 | 33.479 | 42.137 | 1.00 | 29.44 | 6 |
| | ATOM | 1047 | C | LEU | A | 400 | 40.941 | 29.872 | 42.947 | 1.00 | 38.84 | 6 |
| | ATOM | 1048 | O | LEU | A | 400 | 41.367 | 29.632 | 41.821 | 1.00 | 40.38 | 8 |
| | ATOM | 1049 | N | LEU | A | 401 | 41.464 | 29.350 | 44.055 | 1.00 | 42.79 | 7 |
| 10 | ATOM | 1050 | CA | LEU | A | 401 | 42.605 | 28.449 | 43.988 | 1.00 | 43.48 | 6 |
| | ATOM | 1051 | CB | LEU | A | 401 | 42.900 | 27.821 | 45.355 | 1.00 | 44.73 | 6 |
| | ATOM | 1052 | CG | LEU | A | 401 | 44.105 | 26.899 | 45.354 | 1.00 | 51.39 | 6 |
| | ATOM | 1053 | CD1 | LEU | A | 401 | 45.374 | 27.749 | 45.143 | 1.00 | 50.11 | 6 |
| | ATOM | 1054 | CD2 | LEU | A | 401 | 44.205 | 26.122 | 46.662 | 1.00 | 49.30 | 6 |
| 15 | ATOM | 1055 | C | LEU | A | 401 | 42.324 | 27.340 | 42.981 | 1.00 | 41.62 | 6 |
| | ATOM | 1056 | O | LEU | A | 401 | 43.052 | 27.180 | 42.004 | 1.00 | 45.14 | 8 |
| | ATOM | 1057 | N | ALA | A | 402 | 41.269 | 26.574 | 43.245 | 1.00 | 37.92 | 7 |
| | ATOM | 1058 | CA | ALA | A | 402 | 40.873 | 25.469 | 42.386 | 1.00 | 29.90 | 6 |
| | ATOM | 1059 | CB | ALA | A | 402 | 39.522 | 24.928 | 42.834 | 1.00 | 30.70 | 6 |
| 20 | ATOM | 1060 | C | ALA | A | 402 | 40.798 | 25.909 | 40.929 | 1.00 | 28.88 | 6 |
| | ATOM | 1061 | O | ALA | A | 402 | 41.277 | 25.203 | 40.034 | 1.00 | 32.14 | 8 |
| | ATOM | 1062 | N | PHE | A | 403 | 40.200 | 27.086 | 40.707 | 1.00 | 31.07 | 7 |
| | ATOM | 1063 | CA | PHE | A | 403 | 40.052 | 27.642 | 39.363 | 1.00 | 29.90 | 6 |
| | ATOM | 1064 | CB | PHE | A | 403 | 39.379 | 29.019 | 39.438 | 1.00 | 27.03 | 6 |
| 25 | ATOM | 1065 | CG | PHE | A | 403 | 38.943 | 29.574 | 38.100 | 1.00 | 26.97 | 6 |
| | ATOM | 1066 | CD1 | PHE | A | 403 | 38.228 | 30.758 | 38.033 | 1.00 | 25.55 | 6 |
| | ATOM | 1067 | CD2 | PHE | A | 403 | 39.224 | 28.905 | 36.925 | 1.00 | 19.75 | 6 |
| | ATOM | 1068 | CE1 | PHE | A | 403 | 37.784 | 31.266 | 36.808 | 1.00 | 27.90 | 6 |
| | ATOM | 1069 | CE2 | PHE | A | 403 | 38.780 | 29.416 | 35.694 | 1.00 | 22.56 | 6 |
| 30 | ATOM | 1070 | CZ | PHE | A | 403 | 38.063 | 30.596 | 35.640 | 1.00 | 22.24 | 6 |
| | ATOM | 1071 | C | PHE | A | 403 | 41.429 | 27.756 | 38.719 | 1.00 | 28.82 | 6 |
| | ATOM | 1072 | O | PHE | A | 403 | 41.666 | 27.210 | 37.646 | 1.00 | 26.00 | 8 |
| | ATOM | 1073 | N | GLU | A | 404 | 42.329 | 28.463 | 39.402 | 1.00 | 30.25 | 7 |
| | ATOM | 1074 | CA | GLU | A | 404 | 43.695 | 28.665 | 38.922 | 1.00 | 34.03 | 6 |
| 35 | ATOM | 1075 | CB | GLU | A | 404 | 44.513 | 29.416 | 39.983 | 1.00 | 39.45 | 6 |
| | ATOM | 1076 | CG | GLU | A | 404 | 45.867 | 29.935 | 39.489 | 1.00 | 47.68 | 6 |
| | ATOM | 1077 | CD | GLU | A | 404 | 46.734 | 30.507 | 40.571 | 1.00 | 54.02 | 6 |
| | ATOM | 1078 | OE1 | GLU | A | 404 | 46.236 | 31.298 | 41.408 | 1.00 | 57.27 | 8 |
| | ATOM | 1079 | OE2 | GLU | A | 404 | 47.956 | 30.202 | 40.606 | 1.00 | 63.85 | 8 |
| 40 | ATOM | 1080 | C | GLU | A | 404 | 44.352 | 27.322 | 38.634 | 1.00 | 36.01 | 6 |
| | ATOM | 1081 | O | GLU | A | 404 | 44.936 | 27.112 | 37.574 | 1.00 | 38.64 | 8 |
| | ATOM | 1082 | N | HIS | A | 405 | 44.259 | 26.420 | 39.610 | 1.00 | 29.56 | 7 |
| | ATOM | 1083 | CA | HIS | A | 405 | 44.840 | 25.093 | 39.468 | 1.00 | 31.69 | 6 |
| | ATOM | 1084 | CB | HIS | A | 405 | 44.540 | 24.228 | 40.694 | 1.00 | 33.75 | 6 |
| 45 | ATOM | 1085 | CG | HIS | A | 405 | 45.292 | 24.657 | 41.908 | 1.00 | 34.75 | 6 |
| | ATOM | 1086 | CD2 | HIS | A | 405 | 46.198 | 25.640 | 42.130 | 1.00 | 34.58 | 6 |
| | ATOM | 1087 | ND1 | HIS | A | 405 | 45.161 | 23.984 | 43.130 | 1.00 | 32.43 | 7 |
| | ATOM | 1088 | CE1 | HIS | A | 405 | 45.975 | 24.568 | 44.018 | 1.00 | 36.15 | 6 |
| | ATOM | 1089 | NE2 | HIS | A | 405 | 46.601 | 25.561 | 43.430 | 1.00 | 39.84 | 7 |
| 50 | ATOM | 1090 | C | HIS | A | 405 | 44.274 | 24.445 | 38.225 | 1.00 | 34.21 | 6 |
| | ATOM | 1091 | O | HIS | A | 405 | 45.029 | 23.949 | 37.386 | 1.00 | 37.06 | 8 |
| | ATOM | 1092 | N | TYR | A | 406 | 42.947 | 24.453 | 38.100 | 1.00 | 30.83 | 7 |
| | ATOM | 1093 | CA | TYR | A | 406 | 42.313 | 23.859 | 36.930 | 1.00 | 28.85 | 6 |
| | ATOM | 1094 | CB | TYR | A | 406 | 40.805 | 24.080 | 36.934 | 1.00 | 31.48 | 6 |
| 55 | ATOM | 1095 | CG | TYR | A | 406 | 40.139 | 23.494 | 35.709 | 1.00 | 23.49 | 6 |
| | ATOM | 1096 | CD1 | TYR | A | 406 | 40.073 | 22.123 | 35.532 | 1.00 | 19.42 | 6 |
| | ATOM | 1097 | CE1 | TYR | A | 406 | 39.517 | 21.577 | 34.382 | 1.00 | 23.80 | 6 |
| | ATOM | 1098 | CD2 | TYR | A | 406 | 39.646 | 24.313 | 34.704 | 1.00 | 21.81 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 1099 | CE2 | TYR | A | 406 | 39.090 | 23.769 | 33.551 | 1.00 | 24.64 | 6 |
| | ATOM | 1100 | CZ | TYR | A | 406 | 39.029 | 22.395 | 33.380 | 1.00 | 21.56 | 6 |
| | ATOM | 1101 | OH | TYR | A | 406 | 38.489 | 21.850 | 32.236 | 1.00 | 24.96 | 8 |
| | ATOM | 1102 | C | TYR | A | 406 | 42.882 | 24.504 | 35.672 | 1.00 | 24.24 | 6 |
| | ATOM | 1103 | O | TYR | A | 406 | 42.958 | 23.872 | 34.621 | 1.00 | 27.08 | 8 |
| 10 | ATOM | 1104 | N | ILE | A | 407 | 43.253 | 25.784 | 35.807 | 1.00 | 25.76 | 7 |
| | ATOM | 1105 | CA | ILE | A | 407 | 43.824 | 26.548 | 34.705 | 1.00 | 33.75 | 6 |
| | ATOM | 1106 | CB | ILE | A | 407 | 43.986 | 28.033 | 35.070 | 1.00 | 34.23 | 6 |
| | ATOM | 1107 | CG2 | ILE | A | 407 | 44.967 | 28.712 | 34.139 | 1.00 | 32.46 | 6 |
| | ATOM | 1108 | CG1 | ILE | A | 407 | 42.615 | 28.728 | 35.042 | 1.00 | 43.30 | 6 |
| 15 | ATOM | 1109 | CD1 | ILE | A | 407 | 41.896 | 28.602 | 33.694 | 1.00 | 40.40 | 6 |
| | ATOM | 1110 | C | ILE | A | 407 | 45.143 | 25.973 | 34.256 | 1.00 | 39.03 | 6 |
| | ATOM | 1111 | O | ILE | A | 407 | 45.383 | 25.771 | 33.063 | 1.00 | 35.18 | 8 |
| | ATOM | 1112 | N | ASN | A | 408 | 46.003 | 25.721 | 35.227 | 1.00 | 37.25 | 7 |
| | ATOM | 1113 | CA | ASN | A | 408 | 47.307 | 25.194 | 34.926 | 1.00 | 37.01 | 6 |
| 20 | ATOM | 1114 | CB | ASN | A | 408 | 48.107 | 25.017 | 36.213 | 1.00 | 32.27 | 6 |
| | ATOM | 1115 | CG | ASN | A | 408 | 48.346 | 26.362 | 36.936 | 1.00 | 33.56 | 6 |
| | ATOM | 1116 | OD1 | ASN | A | 408 | 48.827 | 27.335 | 36.320 | 1.00 | 31.99 | 8 |
| | ATOM | 1117 | ND2 | ASN | A | 408 | 48.038 | 26.403 | 38.231 | 1.00 | 31.23 | 7 |
| | ATOM | 1118 | C | ASN | A | 408 | 47.205 | 23.892 | 34.136 | 1.00 | 38.14 | 6 |
| 25 | ATOM | 1119 | O | ASN | A | 408 | 47.900 | 23.734 | 33.124 | 1.00 | 42.16 | 8 |
| | ATOM | 1120 | N | TYR | A | 409 | 46.334 | 22.981 | 34.568 | 1.00 | 35.62 | 7 |
| | ATOM | 1121 | CA | TYR | A | 409 | 46.159 | 21.710 | 33.866 | 1.00 | 35.91 | 6 |
| | ATOM | 1122 | CB | TYR | A | 409 | 45.051 | 20.859 | 34.507 | 1.00 | 34.41 | 6 |
| | ATOM | 1123 | CG | TYR | A | 409 | 44.624 | 19.687 | 33.619 | 1.00 | 38.73 | 6 |
| 30 | ATOM | 1124 | CD1 | TYR | A | 409 | 45.563 | 18.765 | 33.155 | 1.00 | 41.34 | 6 |
| | ATOM | 1125 | CE1 | TYR | A | 409 | 45.186 | 17.709 | 32.321 | 1.00 | 47.16 | 6 |
| | ATOM | 1126 | CD2 | TYR | A | 409 | 43.292 | 19.515 | 33.232 | 1.00 | 46.20 | 6 |
| | ATOM | 1127 | CE2 | TYR | A | 409 | 42.913 | 18.455 | 32.397 | 1.00 | 50.74 | 6 |
| | ATOM | 1128 | CZ | TYR | A | 409 | 43.863 | 17.551 | 31.946 | 1.00 | 50.88 | 6 |
| 35 | ATOM | 1129 | OH | TYR | A | 409 | 43.498 | 16.514 | 31.130 | 1.00 | 53.14 | 8 |
| | ATOM | 1130 | C | TYR | A | 409 | 45.760 | 21.966 | 32.424 | 1.00 | 38.16 | 6 |
| | ATOM | 1131 | O | TYR | A | 409 | 46.202 | 21.281 | 31.502 | 1.00 | 41.83 | 8 |
| | ATOM | 1132 | N | ARG | A | 410 | 44.872 | 22.943 | 32.272 | 1.00 | 42.25 | 7 |
| | ATOM | 1133 | CA | ARG | A | 410 | 44.345 | 23.332 | 30.984 | 1.00 | 42.83 | 6 |
| 40 | ATOM | 1134 | CB | ARG | A | 410 | 43.311 | 24.427 | 31.195 | 1.00 | 36.83 | 6 |
| | ATOM | 1135 | CG | ARG | A | 410 | 41.994 | 23.979 | 31.795 | 1.00 | 34.32 | 6 |
| | ATOM | 1136 | CD | ARG | A | 410 | 41.073 | 23.504 | 30.675 | 1.00 | 36.62 | 6 |
| | ATOM | 1137 | NE | ARG | A | 410 | 40.888 | 24.550 | 29.685 | 1.00 | 38.64 | 7 |
| | ATOM | 1138 | CZ | ARG | A | 410 | 40.177 | 24.397 | 28.576 | 1.00 | 35.73 | 6 |
| 45 | ATOM | 1139 | NH1 | ARG | A | 410 | 39.572 | 23.230 | 28.348 | 1.00 | 33.17 | 7 |
| | ATOM | 1140 | NH2 | ARG | A | 410 | 40.077 | 25.407 | 27.708 | 1.00 | 32.70 | 7 |
| | ATOM | 1141 | C | ARG | A | 410 | 45.442 | 23.850 | 30.083 | 1.00 | 46.67 | 6 |
| | ATOM | 1142 | O | ARG | A | 410 | 45.467 | 23.591 | 28.882 | 1.00 | 41.78 | 8 |
| | ATOM | 1143 | N | LYS | A | 411 | 46.360 | 24.577 | 30.710 | 1.00 | 52.99 | 7 |
| 50 | ATOM | 1144 | CA | LYS | A | 411 | 47.467 | 25.194 | 30.017 | 1.00 | 58.32 | 6 |
| | ATOM | 1145 | CB | LYS | A | 411 | 48.645 | 24.216 | 29.876 | 1.00 | 64.99 | 6 |
| | ATOM | 1146 | CG | LYS | A | 411 | 48.349 | 22.835 | 29.367 | 1.00 | 70.48 | 6 |
| | ATOM | 1147 | CD | LYS | A | 411 | 49.608 | 21.974 | 29.494 | 1.00 | 77.18 | 6 |
| | ATOM | 1148 | CE | LYS | A | 411 | 49.461 | 20.621 | 28.795 | 1.00 | 84.30 | 6 |
| 55 | ATOM | 1149 | NZ | LYS | A | 411 | 50.740 | 19.828 | 28.857 | 1.00 | 86.48 | 7 |
| | ATOM | 1150 | C | LYS | A | 411 | 47.032 | 25.756 | 28.686 | 1.00 | 56.66 | 6 |
| | ATOM | 1151 | O | LYS | A | 411 | 47.160 | 25.153 | 27.633 | 1.00 | 55.47 | 8 |
| | ATOM | 1152 | N | HIS | A | 412 | 46.458 | 26.943 | 28.823 | 1.00 | 54.67 | 7 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 1153 | CA | HIS | A | 412 | 45.984 | 27.722 | 27.705 | 1.00 | 48.67 | 6 |
| | ATOM | 1154 | CB | HIS | A | 412 | 45.124 | 28.884 | 28.201 | 1.00 | 43.14 | 6 |
| | ATOM | 1155 | CG | HIS | A | 412 | 43.812 | 28.480 | 28.755 | 1.00 | 41.36 | 6 |
| | ATOM | 1156 | CD2 | HIS | A | 412 | 43.429 | 28.064 | 29.987 | 1.00 | 35.44 | 6 |
| | ATOM | 1157 | ND1 | HIS | A | 412 | 42.651 | 28.440 | 27.966 | 1.00 | 38.19 | 7 |
| 10 | ATOM | 1158 | CE1 | HIS | A | 412 | 41.648 | 28.014 | 28.723 | 1.00 | 34.75 | 6 |
| | ATOM | 1159 | NE2 | HIS | A | 412 | 42.094 | 27.780 | 29.942 | 1.00 | 35.52 | 7 |
| | ATOM | 1160 | C | HIS | A | 412 | 47.231 | 28.303 | 27.101 | 1.00 | 46.35 | 6 |
| | ATOM | 1161 | O | HIS | A | 412 | 48.269 | 28.452 | 27.775 | 1.00 | 42.73 | 8 |
| | ATOM | 1162 | N | HIS | A | 413 | 47.116 | 28.696 | 25.839 | 1.00 | 48.92 | 7 |
| 15 | ATOM | 1163 | CA | HIS | A | 413 | 48.234 | 29.290 | 25.146 | 1.00 | 53.15 | 6 |
| | ATOM | 1164 | CB | HIS | A | 413 | 48.404 | 28.666 | 23.755 | 1.00 | 55.27 | 6 |
| | ATOM | 1165 | CG | HIS | A | 413 | 49.326 | 29.446 | 22.886 | 1.00 | 58.77 | 6 |
| | ATOM | 1166 | CD2 | HIS | A | 413 | 49.213 | 30.660 | 22.304 | 1.00 | 61.65 | 6 |
| | ATOM | 1167 | ND1 | HIS | A | 413 | 50.617 | 28.997 | 22.564 | 1.00 | 60.31 | 7 |
| 20 | ATOM | 1168 | CE1 | HIS | A | 413 | 51.214 | 29.924 | 21.828 | 1.00 | 63.01 | 6 |
| | ATOM | 1169 | NE2 | HIS | A | 413 | 50.386 | 30.941 | 21.658 | 1.00 | 62.93 | 7 |
| | ATOM | 1170 | C | HIS | A | 413 | 47.932 | 30.768 | 24.998 | 1.00 | 53.19 | 6 |
| | ATOM | 1171 | O | HIS | A | 413 | 47.639 | 31.301 | 23.934 | 1.00 | 54.93 | 8 |
| | ATOM | 1172 | N | VAL | A | 414 | 47.964 | 31.413 | 26.139 | 1.00 | 53.77 | 7 |
| 25 | ATOM | 1173 | CA | VAL | A | 414 | 47.735 | 32.811 | 26.146 | 1.00 | 51.06 | 6 |
| | ATOM | 1174 | CB | VAL | A | 414 | 46.291 | 33.183 | 26.417 | 1.00 | 51.49 | 6 |
| | ATOM | 1175 | CG1 | VAL | A | 414 | 46.186 | 34.715 | 26.603 | 1.00 | 45.22 | 6 |
| | ATOM | 1176 | CG2 | VAL | A | 414 | 45.419 | 32.732 | 25.263 | 1.00 | 52.67 | 6 |
| | ATOM | 1177 | C | VAL | A | 414 | 48.623 | 33.283 | 27.226 | 1.00 | 54.28 | 6 |
| 30 | ATOM | 1178 | O | VAL | A | 414 | 48.427 | 33.029 | 28.409 | 1.00 | 55.49 | 8 |
| | ATOM | 1179 | N | THR | A | 415 | 49.706 | 33.863 | 26.733 | 1.00 | 56.28 | 7 |
| | ATOM | 1180 | CA | THR | A | 415 | 50.721 | 34.484 | 27.557 | 1.00 | 57.83 | 6 |
| | ATOM | 1181 | CB | THR | A | 415 | 51.268 | 35.675 | 26.758 | 1.00 | 59.64 | 6 |
| | ATOM | 1182 | OG1 | THR | A | 415 | 51.605 | 36.754 | 27.636 | 1.00 | 66.69 | 8 |
| 35 | ATOM | 1183 | CG2 | THR | A | 415 | 50.197 | 36.158 | 25.745 | 1.00 | 59.42 | 6 |
| | ATOM | 1184 | C | THR | A | 415 | 50.146 | 35.049 | 28.879 | 1.00 | 56.98 | 6 |
| | ATOM | 1185 | O | THR | A | 415 | 48.933 | 35.146 | 29.051 | 1.00 | 55.70 | 8 |
| | ATOM | 1186 | N | HIS | A | 416 | 51.068 | 35.330 | 29.795 | 1.00 | 57.44 | 7 |
| | ATOM | 1187 | CA | HIS | A | 416 | 50.808 | 36.011 | 31.047 | 1.00 | 57.34 | 6 |
| 40 | ATOM | 1188 | CB | HIS | A | 416 | 51.346 | 37.422 | 30.708 | 1.00 | 61.35 | 6 |
| | ATOM | 1189 | CG | HIS | A | 416 | 51.872 | 38.237 | 31.821 | 1.00 | 69.78 | 6 |
| | ATOM | 1190 | CD2 | HIS | A | 416 | 53.114 | 38.297 | 32.390 | 1.00 | 71.42 | 6 |
| | ATOM | 1191 | ND1 | HIS | A | 416 | 51.135 | 39.263 | 32.416 | 1.00 | 72.49 | 7 |
| | ATOM | 1192 | CE1 | HIS | A | 416 | 51.914 | 39.884 | 33.290 | 1.00 | 75.50 | 6 |
| 45 | ATOM | 1193 | NE2 | HIS | A | 416 | 53.099 | 39.323 | 33.291 | 1.00 | 73.91 | 7 |
| | ATOM | 1194 | C | HIS | A | 416 | 49.261 | 35.892 | 31.297 | 1.00 | 53.79 | 6 |
| | ATOM | 1195 | O | HIS | A | 416 | 48.499 | 36.779 | 30.902 | 1.00 | 52.81 | 8 |
| | ATOM | 1196 | N | PHE | A | 417 | 48.806 | 34.779 | 31.911 | 1.00 | 48.05 | 7 |
| | ATOM | 1197 | CA | PHE | A | 417 | 47.355 | 34.428 | 32.061 | 1.00 | 47.99 | 6 |
| 50 | ATOM | 1198 | CB | PHE | A | 417 | 47.165 | 32.954 | 31.996 | 1.00 | 46.11 | 6 |
| | ATOM | 1199 | CG | PHE | A | 417 | 45.835 | 32.590 | 31.399 | 1.00 | 44.27 | 6 |
| | ATOM | 1200 | CD1 | PHE | A | 417 | 45.680 | 32.720 | 30.046 | 1.00 | 41.79 | 6 |
| | ATOM | 1201 | CD2 | PHE | A | 417 | 44.758 | 32.135 | 32.164 | 1.00 | 40.23 | 6 |
| | ATOM | 1202 | CE1 | PHE | A | 417 | 44.498 | 32.397 | 29.422 | 1.00 | 44.30 | 6 |
| 55 | ATOM | 1203 | CE2 | PHE | A | 417 | 43.540 | 31.802 | 31.529 | 1.00 | 36.80 | 6 |
| | ATOM | 1204 | CZ | PHE | A | 417 | 43.427 | 31.928 | 30.144 | 1.00 | 40.69 | 6 |
| | ATOM | 1205 | C | PHE | A | 417 | 46.427 | 34.836 | 33.196 | 1.00 | 46.69 | 6 |
| | ATOM | 1206 | O | PHE | A | 417 | 46.147 | 36.004 | 33.331 | 1.00 | 43.35 | 8 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| 5 | ATOM | 1207 | N | TRP | A | 418 | 45.906 | 33.801 | 33.909 | 1.00 | 45.14 | 7 |
| | ATOM | 1208 | CA | TRP | A | 418 | 44.982 | 33.867 | 35.065 | 1.00 | 44.89 | 6 |
| | ATOM | 1209 | CB | TRP | A | 418 | 45.545 | 33.099 | 36.255 | 1.00 | 42.24 | 6 |
| | ATOM | 1210 | CG | TRP | A | 418 | 44.959 | 33.452 | 37.598 | 1.00 | 47.11 | 6 |
| | ATOM | 1211 | CD2 | TRP | A | 418 | 43.724 | 32.924 | 38.149 | 1.00 | 46.98 | 6 |
| 10 | ATOM | 1212 | CE2 | TRP | A | 418 | 43.534 | 33.565 | 39.413 | 1.00 | 48.94 | 6 |
| | ATOM | 1213 | CE3 | TRP | A | 418 | 42.777 | 31.986 | 37.688 | 1.00 | 45.23 | 6 |
| | ATOM | 1214 | CD1 | TRP | A | 418 | 45.434 | 34.350 | 38.512 | 1.00 | 46.24 | 6 |
| | ATOM | 1215 | NE1 | TRP | A | 418 | 44.588 | 34.407 | 39.608 | 1.00 | 50.63 | 7 |
| | ATOM | 1216 | CZ2 | TRP | A | 418 | 42.441 | 33.270 | 40.238 | 1.00 | 45.46 | 6 |
| 15 | ATOM | 1217 | CZ3 | TRP | A | 418 | 41.686 | 31.706 | 38.500 | 1.00 | 44.50 | 6 |
| | ATOM | 1218 | CH2 | TRP | A | 418 | 41.511 | 32.335 | 39.753 | 1.00 | 47.55 | 6 |
| | ATOM | 1219 | C | TRP | A | 418 | 44.908 | 35.324 | 35.398 | 1.00 | 43.88 | 6 |
| | ATOM | 1220 | O | TRP | A | 418 | 43.797 | 35.839 | 35.702 | 1.00 | 43.17 | 8 |
| | ATOM | 1221 | N | PRO | A | 419 | 46.084 | 35.976 | 35.461 | 1.00 | 43.55 | 7 |
| 20 | ATOM | 1222 | CD | PRO | A | 419 | 47.467 | 35.482 | 35.400 | 1.00 | 41.52 | 6 |
| | ATOM | 1223 | CA | PRO | A | 419 | 46.009 | 37.396 | 35.758 | 1.00 | 41.48 | 6 |
| | ATOM | 1224 | CB | PRO | A | 419 | 47.436 | 37.884 | 35.535 | 1.00 | 39.21 | 6 |
| | ATOM | 1225 | CG | PRO | A | 419 | 48.261 | 36.696 | 35.223 | 1.00 | 39.25 | 6 |
| | ATOM | 1226 | C | PRO | A | 419 | 44.960 | 38.090 | 34.817 | 1.00 | 36.28 | 6 |
| 25 | ATOM | 1227 | O | PRO | A | 419 | 44.208 | 38.978 | 35.237 | 1.00 | 37.08 | 8 |
| | ATOM | 1228 | N | LYS | A | 420 | 44.915 | 37.701 | 33.540 | 1.00 | 35.96 | 7 |
| | ATOM | 1229 | CA | LYS | A | 420 | 43.977 | 38.287 | 32.575 | 1.00 | 40.82 | 6 |
| | ATOM | 1230 | CB | LYS | A | 420 | 44.314 | 37.805 | 31.155 | 1.00 | 40.78 | 6 |
| | ATOM | 1231 | CG | LYS | A | 420 | 45.684 | 38.244 | 30.641 | 1.00 | 48.62 | 6 |
| 30 | ATOM | 1232 | CD | LYS | A | 420 | 45.904 | 37.781 | 29.206 | 1.00 | 55.12 | 6 |
| | ATOM | 1233 | CE | LYS | A | 420 | 47.248 | 38.261 | 28.673 | 1.00 | 53.26 | 6 |
| | ATOM | 1234 | NZ | LYS | A | 420 | 47.448 | 37.884 | 27.222 | 1.00 | 52.69 | 7 |
| | ATOM | 1235 | C | LYS | A | 420 | 42.580 | 37.832 | 32.948 | 1.00 | 40.29 | 6 |
| | ATOM | 1236 | O | LYS | A | 420 | 41.656 | 38.626 | 32.982 | 1.00 | 39.66 | 8 |
| 35 | ATOM | 1237 | N | LEU | A | 421 | 42.461 | 36.537 | 33.245 | 1.00 | 38.33 | 7 |
| | ATOM | 1238 | CA | LEU | A | 421 | 41.186 | 35.931 | 33.613 | 1.00 | 37.60 | 6 |
| | ATOM | 1239 | CB | LEU | A | 421 | 41.397 | 34.433 | 33.915 | 1.00 | 43.66 | 6 |
| | ATOM | 1240 | CG | LEU | A | 421 | 40.204 | 33.518 | 33.828 | 1.00 | 46.50 | 6 |
| | ATOM | 1241 | CD1 | LEU | A | 421 | 39.643 | 33.624 | 32.426 | 1.00 | 45.15 | 6 |
| 40 | ATOM | 1242 | CD2 | LEU | A | 421 | 40.595 | 32.094 | 34.131 | 1.00 | 51.31 | 6 |
| | ATOM | 1243 | C | LEU | A | 421 | 40.575 | 36.664 | 34.808 | 1.00 | 39.59 | 6 |
| | ATOM | 1244 | O | LEU | A | 421 | 39.371 | 36.910 | 34.837 | 1.00 | 40.66 | 8 |
| | ATOM | 1245 | N | LEU | A | 422 | 41.412 | 37.017 | 35.782 | 1.00 | 39.57 | 7 |
| | ATOM | 1246 | CA | LEU | A | 422 | 40.946 | 37.726 | 36.961 | 1.00 | 38.63 | 6 |
| 45 | ATOM | 1247 | CB | LEU | A | 422 | 42.085 | 37.890 | 37.971 | 1.00 | 41.79 | 6 |
| | ATOM | 1248 | CG | LEU | A | 422 | 42.424 | 36.671 | 38.798 | 1.00 | 42.74 | 6 |
| | ATOM | 1249 | CD1 | LEU | A | 422 | 43.490 | 37.010 | 39.820 | 1.00 | 42.89 | 6 |
| | ATOM | 1250 | CD2 | LEU | A | 422 | 41.168 | 36.216 | 39.523 | 1.00 | 39.27 | 6 |
| | ATOM | 1251 | C | LEU | A | 422 | 40.381 | 39.073 | 36.589 | 1.00 | 40.47 | 6 |
| 50 | ATOM | 1252 | O | LEU | A | 422 | 39.428 | 39.525 | 37.210 | 1.00 | 47.83 | 8 |
| | ATOM | 1253 | N | MET | A | 423 | 40.969 | 39.698 | 35.569 | 1.00 | 34.27 | 7 |
| | ATOM | 1254 | CA | MET | A | 423 | 40.511 | 41.001 | 35.117 | 1.00 | 35.25 | 6 |
| | ATOM | 1255 | CB | MET | A | 423 | 41.427 | 41.553 | 34.028 | 1.00 | 32.56 | 6 |
| | ATOM | 1256 | CG | MET | A | 423 | 42.856 | 41.732 | 34.456 | 1.00 | 40.70 | 6 |
| 55 | ATOM | 1257 | SD | MET | A | 423 | 43.707 | 43.101 | 33.619 | 1.00 | 47.65 | 16 |
| | ATOM | 1258 | CE | MET | A | 423 | 43.348 | 42.776 | 31.848 | 1.00 | 47.16 | 6 |
| | ATOM | 1259 | C | MET | A | 423 | 39.100 | 40.899 | 34.574 | 1.00 | 35.13 | 6 |
| | ATOM | 1260 | O | MET | A | 423 | 38.315 | 41.829 | 34.696 | 1.00 | 29.85 | 8 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 1261 | N | LYS | A | 424 | 38.791 | 39.752 | 33.975 | 1.00 | 31.56 | 7 |
| | ATOM | 1262 | CA | LYS | A | 424 | 37.470 | 39.529 | 33.423 | 1.00 | 32.29 | 6 |
| | ATOM | 1263 | CB | LYS | A | 424 | 37.446 | 38.205 | 32.658 | 1.00 | 30.56 | 6 |
| | ATOM | 1264 | CG | LYS | A | 424 | 38.394 | 38.192 | 31.455 | 1.00 | 30.07 | 6 |
| | ATOM | 1265 | CD | LYS | A | 424 | 38.050 | 39.326 | 30.488 | 1.00 | 33.22 | 6 |
| 10 | ATOM | 1266 | CE | LYS | A | 424 | 39.032 | 39.433 | 29.322 | 1.00 | 28.75 | 6 |
| | ATOM | 1267 | NZ | LYS | A | 424 | 40.394 | 39.942 | 29.707 | 1.00 | 31.01 | 7 |
| | ATOM | 1268 | C | LYS | A | 424 | 36.418 | 39.558 | 34.524 | 1.00 | 29.26 | 6 |
| | ATOM | 1269 | O | LYS | A | 424 | 35.307 | 39.998 | 34.289 | 1.00 | 30.22 | 8 |
| | ATOM | 1270 | N | VAL | A | 425 | 36.796 | 39.098 | 35.719 | 1.00 | 23.53 | 7 |
| 15 | ATOM | 1271 | CA | VAL | A | 425 | 35.897 | 39.107 | 36.866 | 1.00 | 28.91 | 6 |
| | ATOM | 1272 | CB | VAL | A | 425 | 36.541 | 38.460 | 38.094 | 1.00 | 29.44 | 6 |
| | ATOM | 1273 | CG1 | VAL | A | 425 | 35.673 | 38.642 | 39.320 | 1.00 | 28.81 | 6 |
| | ATOM | 1274 | CG2 | VAL | A | 425 | 36.764 | 36.985 | 37.849 | 1.00 | 31.22 | 6 |
| | ATOM | 1275 | C | VAL | A | 425 | 35.512 | 40.548 | 37.161 | 1.00 | 32.03 | 6 |
| 20 | ATOM | 1276 | O | VAL | A | 425 | 34.350 | 40.839 | 37.429 | 1.00 | 31.95 | 8 |
| | ATOM | 1277 | N | THR | A | 426 | 36.496 | 41.444 | 37.124 | 1.00 | 33.61 | 7 |
| | ATOM | 1278 | CA | THR | A | 426 | 36.248 | 42.866 | 37.356 | 1.00 | 30.76 | 6 |
| | ATOM | 1279 | CB | THR | A | 426 | 37.559 | 43.670 | 37.360 | 1.00 | 32.34 | 6 |
| | ATOM | 1280 | OG1 | THR | A | 426 | 38.209 | 43.565 | 38.630 | 1.00 | 33.07 | 8 |
| 25 | ATOM | 1281 | CG2 | THR | A | 426 | 37.302 | 45.131 | 37.015 | 1.00 | 25.40 | 6 |
| | ATOM | 1282 | C | THR | A | 426 | 35.363 | 43.324 | 36.211 | 1.00 | 32.53 | 6 |
| | ATOM | 1283 | O | THR | A | 426 | 34.357 | 44.006 | 36.405 | 1.00 | 35.19 | 8 |
| | ATOM | 1284 | N | ASP | A | 427 | 35.763 | 42.929 | 35.006 | 1.00 | 28.83 | 7 |
| | ATOM | 1285 | CA | ASP | A | 427 | 35.011 | 43.272 | 33.810 | 1.00 | 35.12 | 6 |
| 30 | ATOM | 1286 | CB | ASP | A | 427 | 35.556 | 42.524 | 32.578 | 1.00 | 39.14 | 6 |
| | ATOM | 1287 | CG | ASP | A | 427 | 36.837 | 43.103 | 32.057 | 1.00 | 45.80 | 6 |
| | ATOM | 1288 | OD1 | ASP | A | 427 | 36.982 | 44.346 | 32.024 | 1.00 | 41.97 | 8 |
| | ATOM | 1289 | OD2 | ASP | A | 427 | 37.735 | 42.333 | 31.616 | 1.00 | 50.06 | 8 |
| | ATOM | 1290 | C | ASP | A | 427 | 33.537 | 42.925 | 34.028 | 1.00 | 33.94 | 6 |
| 35 | ATOM | 1291 | O | ASP | A | 427 | 32.659 | 43.712 | 33.702 | 1.00 | 38.02 | 8 |
| | ATOM | 1292 | N | LEU | A | 428 | 33.283 | 41.745 | 34.584 | 1.00 | 27.15 | 7 |
| | ATOM | 1293 | CA | LEU | A | 428 | 31.925 | 41.293 | 34.850 | 1.00 | 29.99 | 6 |
| | ATOM | 1294 | CB | LEU | A | 428 | 31.924 | 39.786 | 35.133 | 1.00 | 22.49 | 6 |
| | ATOM | 1295 | CG | LEU | A | 428 | 32.104 | 38.873 | 33.939 | 1.00 | 25.54 | 6 |
| 40 | ATOM | 1296 | CD1 | LEU | A | 428 | 32.202 | 37.421 | 34.353 | 1.00 | 20.60 | 6 |
| | ATOM | 1297 | CD2 | LEU | A | 428 | 30.920 | 39.083 | 33.029 | 1.00 | 17.24 | 6 |
| | ATOM | 1298 | C | LEU | A | 428 | 31.276 | 42.057 | 35.991 | 1.00 | 28.94 | 6 |
| | ATOM | 1299 | O | LEU | A | 428 | 30.082 | 42.306 | 35.939 | 1.00 | 31.26 | 8 |
| | ATOM | 1300 | N | ARG | A | 429 | 32.059 | 42.423 | 37.011 | 1.00 | 27.64 | 7 |
| 45 | ATOM | 1301 | CA | ARG | A | 429 | 31.527 | 43.162 | 38.147 | 1.00 | 28.13 | 6 |
| | ATOM | 1302 | CB | ARG | A | 429 | 32.564 | 43.298 | 39.264 | 1.00 | 29.59 | 6 |
| | ATOM | 1303 | CG | ARG | A | 429 | 32.818 | 42.040 | 40.080 | 1.00 | 34.85 | 6 |
| | ATOM | 1304 | CD | ARG | A | 429 | 33.588 | 42.360 | 41.367 | 1.00 | 47.18 | 6 |
| | ATOM | 1305 | NE | ARG | A | 429 | 34.093 | 41.175 | 42.049 | 1.00 | 57.93 | 7 |
| 50 | ATOM | 1306 | CZ | ARG | A | 429 | 33.327 | 40.210 | 42.547 | 1.00 | 63.62 | 6 |
| | ATOM | 1307 | NH1 | ARG | A | 429 | 31.998 | 40.270 | 42.396 | 1.00 | 60.71 | 7 |
| | ATOM | 1308 | NH2 | ARG | A | 429 | 33.900 | 39.165 | 43.150 | 1.00 | 62.38 | 7 |
| | ATOM | 1309 | C | ARG | A | 429 | 31.099 | 44.536 | 37.707 | 1.00 | 29.81 | 6 |
| | ATOM | 1310 | O | ARG | A | 429 | 30.044 | 45.009 | 38.101 | 1.00 | 30.81 | 8 |
| 55 | ATOM | 1311 | N | MET | A | 430 | 31.941 | 45.176 | 36.901 | 1.00 | 29.64 | 7 |
| | ATOM | 1312 | CA | MET | A | 430 | 31.644 | 46.502 | 36.383 | 1.00 | 34.72 | 6 |
| | ATOM | 1313 | CB | MET | A | 430 | 32.745 | 46.955 | 35.434 | 1.00 | 34.97 | 6 |
| | ATOM | 1314 | CG | MET | A | 430 | 33.937 | 47.597 | 36.080 | 1.00 | 45.34 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| 5 | ATOM | 1315 | SD | MET | A | 430 | 33.520 | 49.120 | 36.937 | 1.00 | 52.55 | 16 |
| | ATOM | 1316 | CE | MET | A | 430 | 32.942 | 50.174 | 35.585 | 1.00 | 55.56 | 6 |
| | ATOM | 1317 | C | MET | A | 430 | 30.315 | 46.455 | 35.634 | 1.00 | 34.01 | 6 |
| | ATOM | 1318 | O | MET | A | 430 | 29.455 | 47.295 | 35.854 | 1.00 | 37.29 | 8 |
| | ATOM | 1319 | N | ILE | A | 431 | 30.180 | 45.468 | 34.740 | 1.00 | 29.99 | 7 |
| 10 | ATOM | 1320 | CA | ILE | A | 431 | 28.954 | 45.269 | 33.969 | 1.00 | 28.82 | 6 |
| | ATOM | 1321 | CB | ILE | A | 431 | 28.962 | 43.936 | 33.211 | 1.00 | 27.39 | 6 |
| | ATOM | 1322 | CG2 | ILE | A | 431 | 27.622 | 43.671 | 32.572 | 1.00 | 23.87 | 6 |
| | ATOM | 1323 | CG1 | ILE | A | 431 | 30.044 | 43.920 | 32.138 | 1.00 | 25.56 | 6 |
| | ATOM | 1324 | CD1 | ILE | A | 431 | 29.989 | 42.703 | 31.244 | 1.00 | 17.29 | 6 |
| 15 | ATOM | 1325 | C | ILE | A | 431 | 27.769 | 45.269 | 34.907 | 1.00 | 29.49 | 6 |
| | ATOM | 1326 | O | ILE | A | 431 | 26.810 | 45.993 | 34.712 | 1.00 | 24.19 | 8 |
| | ATOM | 1327 | N | GLY | A | 432 | 27.839 | 44.435 | 35.936 | 1.00 | 25.25 | 7 |
| | ATOM | 1328 | CA | GLY | A | 432 | 26.748 | 44.343 | 36.890 | 1.00 | 30.38 | 6 |
| | ATOM | 1329 | C | GLY | A | 432 | 26.494 | 45.671 | 37.554 | 1.00 | 32.75 | 6 |
| 20 | ATOM | 1330 | O | GLY | A | 432 | 25.411 | 46.206 | 37.469 | 1.00 | 36.38 | 8 |
| | ATOM | 1331 | N | ALA | A | 433 | 27.514 | 46.189 | 38.221 | 1.00 | 26.77 | 7 |
| | ATOM | 1332 | CA | ALA | A | 433 | 27.428 | 47.459 | 38.910 | 1.00 | 26.48 | 6 |
| | ATOM | 1333 | CB | ALA | A | 433 | 28.836 | 47.970 | 39.203 | 1.00 | 19.90 | 6 |
| | ATOM | 1334 | C | ALA | A | 433 | 26.663 | 48.502 | 38.114 | 1.00 | 30.73 | 6 |
| 25 | ATOM | 1335 | O | ALA | A | 433 | 25.773 | 49.164 | 38.635 | 1.00 | 31.60 | 8 |
| | ATOM | 1336 | N | CYS | A | 434 | 27.027 | 48.654 | 36.854 | 1.00 | 33.22 | 7 |
| | ATOM | 1337 | CA | CYS | A | 434 | 26.371 | 49.616 | 35.996 | 1.00 | 34.34 | 6 |
| | ATOM | 1338 | CB | CYS | A | 434 | 27.047 | 49.612 | 34.711 | 1.00 | 35.20 | 6 |
| | ATOM | 1339 | SG | CYS | A | 434 | 27.789 | 50.811 | 34.285 | 1.00 | 54.48 | 16 |
| 30 | ATOM | 1340 | C | CYS | A | 434 | 24.974 | 49.198 | 35.612 | 1.00 | 34.09 | 6 |
| | ATOM | 1341 | O | CYS | A | 434 | 24.107 | 50.040 | 35.415 | 1.00 | 34.89 | 8 |
| | ATOM | 1342 | N | HIS | A | 435 | 24.756 | 47.898 | 35.447 | 1.00 | 34.30 | 7 |
| | ATOM | 1343 | CA | HIS | A | 435 | 23.453 | 47.423 | 35.042 | 1.00 | 35.44 | 6 |
| | ATOM | 1344 | CB | HIS | A | 435 | 23.404 | 45.904 | 35.104 | 1.00 | 31.76 | 6 |
| 35 | ATOM | 1345 | CG | HIS | A | 435 | 22.099 | 45.351 | 34.675 | 1.00 | 32.03 | 6 |
| | ATOM | 1346 | CD2 | HIS | A | 435 | 21.697 | 44.790 | 33.519 | 1.00 | 28.61 | 6 |
| | ATOM | 1347 | ND1 | HIS | A | 435 | 20.941 | 45.482 | 35.452 | 1.00 | 28.48 | 7 |
| | ATOM | 1348 | CE1 | HIS | A | 435 | 19.912 | 45.025 | 34.759 | 1.00 | 33.27 | 6 |
| | ATOM | 1349 | NE2 | HIS | A | 435 | 20.345 | 44.597 | 33.583 | 1.00 | 31.57 | 7 |
| 40 | ATOM | 1350 | C | HIS | A | 435 | 22.400 | 47.974 | 35.972 | 1.00 | 32.74 | 6 |
| | ATOM | 1351 | O | HIS | A | 435 | 21.304 | 48.284 | 35.565 | 1.00 | 32.87 | 8 |
| | ATOM | 1352 | N | ALA | A | 436 | 22.777 | 48.046 | 37.241 | 1.00 | 31.01 | 7 |
| | ATOM | 1353 | CA | ALA | A | 436 | 21.910 | 48.563 | 38.266 | 1.00 | 29.91 | 6 |
| | ATOM | 1354 | CB | ALA | A | 436 | 22.661 | 48.595 | 39.580 | 1.00 | 21.23 | 6 |
| 45 | ATOM | 1355 | C | ALA | A | 436 | 21.475 | 49.969 | 37.884 | 1.00 | 33.86 | 6 |
| | ATOM | 1356 | O | ALA | A | 436 | 20.296 | 50.298 | 37.910 | 1.00 | 36.10 | 8 |
| | ATOM | 1357 | N | SER | A | 437 | 22.453 | 50.795 | 37.532 | 1.00 | 35.19 | 7 |
| | ATOM | 1358 | CA | SER | A | 437 | 22.172 | 52.167 | 37.140 | 1.00 | 33.03 | 6 |
| | ATOM | 1359 | CB | SER | A | 437 | 23.441 | 52.815 | 36.603 | 1.00 | 35.31 | 6 |
| 50 | ATOM | 1360 | OG | SER | A | 437 | 23.203 | 54.151 | 36.193 | 1.00 | 44.99 | 8 |
| | ATOM | 1361 | C | SER | A | 437 | 21.110 | 52.158 | 36.055 | 1.00 | 38.39 | 6 |
| | ATOM | 1362 | O | SER | A | 437 | 20.049 | 52.745 | 36.204 | 1.00 | 37.54 | 8 |
| | ATOM | 1363 | N | ARG | A | 438 | 21.432 | 51.483 | 34.956 | 1.00 | 37.32 | 7 |
| | ATOM | 1364 | CA | ARG | A | 438 | 20.534 | 51.379 | 33.821 | 1.00 | 39.30 | 6 |
| 55 | ATOM | 1365 | CB | ARG | A | 438 | 21.114 | 50.402 | 32.786 | 1.00 | 42.97 | 6 |
| | ATOM | 1366 | CG | ARG | A | 438 | 22.343 | 50.911 | 32.051 | 1.00 | 41.72 | 6 |
| | ATOM | 1367 | CD | ARG | A | 438 | 21.955 | 52.134 | 31.251 | 1.00 | 45.23 | 6 |
| | ATOM | 1368 | NE | ARG | A | 438 | 20.964 | 51.839 | 30.237 | 1.00 | 45.66 | 7 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| 5 | ATOM | 1369 | CZ | ARG | A | 438 | 20.063 | 52.718 | 29.809 | 1.00 | 49.71 | 6 |
| | ATOM | 1370 | NH1 | ARG | A | 438 | 20.046 | 53.958 | 30.318 | 1.00 | 50.91 | 7 |
| | ATOM | 1371 | NH2 | ARG | A | 438 | 19.198 | 52.354 | 28.865 | 1.00 | 46.86 | 7 |
| | ATOM | 1372 | C | ARG | A | 438 | 19.147 | 50.922 | 34.240 | 1.00 | 42.37 | 6 |
| | ATOM | 1373 | O | ARG | A | 438 | 18.147 | 51.297 | 33.625 | 1.00 | 40.58 | 8 |
| 10 | ATOM | 1374 | N | PHE | A | 439 | 19.080 | 50.120 | 35.298 | 1.00 | 42.25 | 7 |
| | ATOM | 1375 | CA | PHE | A | 439 | 17.803 | 49.624 | 35.763 | 1.00 | 42.81 | 6 |
| | ATOM | 1376 | CB | PHE | A | 439 | 17.975 | 48.794 | 37.013 | 1.00 | 42.18 | 6 |
| | ATOM | 1377 | CG | PHE | A | 439 | 16.739 | 48.053 | 37.413 | 1.00 | 42.48 | 6 |
| | ATOM | 1378 | CD1 | PHE | A | 439 | 16.198 | 47.111 | 36.562 | 1.00 | 47.09 | 6 |
| 15 | ATOM | 1379 | CD2 | PHE | A | 439 | 16.105 | 48.320 | 38.613 | 1.00 | 39.76 | 6 |
| | ATOM | 1380 | CE1 | PHE | A | 439 | 15.047 | 46.427 | 36.905 | 1.00 | 49.17 | 6 |
| | ATOM | 1381 | CE2 | PHE | A | 439 | 14.940 | 47.630 | 38.963 | 1.00 | 45.10 | 6 |
| | ATOM | 1382 | CZ | PHE | A | 439 | 14.411 | 46.683 | 38.098 | 1.00 | 46.36 | 6 |
| | ATOM | 1383 | C | PHE | A | 439 | 16.921 | 50.803 | 36.075 | 1.00 | 44.79 | 6 |
| 20 | ATOM | 1384 | O | PHE | A | 439 | 15.830 | 50.903 | 35.554 | 1.00 | 40.26 | 8 |
| | ATOM | 1385 | N | LEU | A | 440 | 17.410 | 51.681 | 36.951 | 1.00 | 42.77 | 7 |
| | ATOM | 1386 | CA | LEU | A | 440 | 16.660 | 52.871 | 37.344 | 1.00 | 42.96 | 6 |
| | ATOM | 1387 | CB | LEU | A | 440 | 17.546 | 53.824 | 38.150 | 1.00 | 37.19 | 6 |
| | ATOM | 1388 | CG | LEU | A | 440 | 17.943 | 53.297 | 39.500 | 1.00 | 36.97 | 6 |
| 25 | ATOM | 1389 | CD1 | LEU | A | 440 | 18.620 | 54.389 | 40.316 | 1.00 | 33.65 | 6 |
| | ATOM | 1390 | CD2 | LEU | A | 440 | 16.679 | 52.837 | 40.216 | 1.00 | 35.42 | 6 |
| | ATOM | 1391 | C | LEU | A | 440 | 16.025 | 53.596 | 36.168 | 1.00 | 45.47 | 6 |
| | ATOM | 1392 | O | LEU | A | 440 | 14.809 | 53.750 | 36.126 | 1.00 | 52.48 | 8 |
| | ATOM | 1393 | N | HIS | A | 441 | 16.836 | 54.060 | 35.223 | 1.00 | 49.15 | 7 |
| 30 | ATOM | 1394 | CA | HIS | A | 441 | 16.277 | 54.725 | 34.063 | 1.00 | 54.76 | 6 |
| | ATOM | 1395 | CB | HIS | A | 441 | 17.329 | 54.955 | 33.031 | 1.00 | 56.68 | 6 |
| | ATOM | 1396 | CG | HIS | A | 441 | 18.134 | 56.161 | 33.282 | 1.00 | 62.73 | 6 |
| | ATOM | 1397 | CD2 | HIS | A | 441 | 18.468 | 57.216 | 32.499 | 1.00 | 65.73 | 6 |
| | ATOM | 1398 | ND1 | HIS | A | 441 | 18.701 | 56.431 | 34.538 | 1.00 | 66.01 | 7 |
| 35 | ATOM | 1399 | CE1 | HIS | A | 441 | 19.332 | 57.594 | 34.473 | 1.00 | 65.55 | 6 |
| | ATOM | 1400 | NE2 | HIS | A | 441 | 19.205 | 58.085 | 33.255 | 1.00 | 60.09 | 7 |
| | ATOM | 1401 | C | HIS | A | 441 | 15.244 | 53.822 | 33.481 | 1.00 | 55.93 | 6 |
| | ATOM | 1402 | O | HIS | A | 441 | 14.149 | 54.263 | 33.170 | 1.00 | 57.33 | 8 |
| | ATOM | 1403 | N | MET | A | 442 | 15.605 | 52.549 | 33.313 | 1.00 | 57.81 | 7 |
| 40 | ATOM | 1404 | CA | MET | A | 442 | 14.661 | 51.583 | 32.778 | 1.00 | 59.11 | 6 |
| | ATOM | 1405 | CB | MET | A | 442 | 15.191 | 50.154 | 32.922 | 1.00 | 55.93 | 6 |
| | ATOM | 1406 | CG | MET | A | 442 | 16.336 | 49.813 | 32.022 | 1.00 | 58.52 | 6 |
| | ATOM | 1407 | SD | MET | A | 442 | 16.681 | 48.008 | 31.851 | 1.00 | 60.99 | 16 |
| | ATOM | 1408 | CE | MET | A | 442 | 17.085 | 47.602 | 33.581 | 1.00 | 52.61 | 6 |
| 45 | ATOM | 1409 | C | MET | A | 442 | 13.339 | 51.727 | 33.534 | 1.00 | 60.31 | 6 |
| | ATOM | 1410 | O | MET | A | 442 | 12.266 | 51.560 | 32.968 | 1.00 | 58.18 | 8 |
| | ATOM | 1411 | N | LYS | A | 443 | 13.425 | 52.054 | 34.818 | 1.00 | 61.45 | 7 |
| | ATOM | 1412 | CA | LYS | A | 443 | 12.236 | 52.202 | 35.626 | 1.00 | 64.90 | 6 |
| | ATOM | 1413 | CB | LYS | A | 443 | 12.608 | 52.141 | 37.090 | 1.00 | 64.40 | 6 |
| 50 | ATOM | 1414 | CG | LYS | A | 443 | 11.461 | 51.748 | 37.959 | 1.00 | 69.12 | 6 |
| | ATOM | 1415 | CD | LYS | A | 443 | 12.068 | 51.551 | 39.257 | 1.00 | 71.14 | 6 |
| | ATOM | 1416 | CE | LYS | A | 443 | 11.368 | 51.897 | 40.091 | 1.00 | 73.43 | 6 |
| | ATOM | 1417 | NZ | LYS | A | 443 | 11.883 | 51.712 | 41.415 | 1.00 | 67.97 | 7 |
| | ATOM | 1418 | C | LYS | A | 443 | 11.513 | 53.514 | 35.348 | 1.00 | 67.29 | 6 |
| 55 | ATOM | 1419 | O | LYS | A | 443 | 10.390 | 53.700 | 35.780 | 1.00 | 67.90 | 8 |
| | ATOM | 1420 | N | VAL | A | 444 | 12.171 | 54.429 | 34.629 | 1.00 | 66.57 | 7 |
| | ATOM | 1421 | CA | VAL | A | 444 | 11.575 | 55.719 | 34.297 | 1.00 | 64.76 | 6 |
| | ATOM | 1422 | CB | VAL | A | 444 | 12.569 | 56.869 | 34.560 | 1.00 | 62.76 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| 5 | ATOM | 1423 | CG1 | VAL | A | 444 | 11.952 | 58.195 | 34.174 | 1.00 | 64.00 | 6 |
| | ATOM | 1424 | CG2 | VAL | A | 444 | 12.999 | 56.891 | 36.035 | 1.00 | 59.27 | 6 |
| | ATOM | 1425 | C | VAL | A | 444 | 11.043 | 55.730 | 32.861 | 1.00 | 68.61 | 6 |
| | ATOM | 1426 | O | VAL | A | 444 | 9.937 | 56.210 | 32.612 | 1.00 | 70.60 | 8 |
| | ATOM | 1427 | N | GLU | A | 445 | 11.814 | 55.173 | 31.935 | 1.00 | 70.71 | 7 |
| 10 | ATOM | 1428 | CA | GLU | A | 445 | 11.457 | 55.152 | 30.514 | 1.00 | 71.45 | 6 |
| | ATOM | 1429 | CB | GLU | A | 445 | 12.725 | 55.255 | 29.664 | 1.00 | 72.36 | 6 |
| | ATOM | 1430 | CG | GLU | A | 445 | 13.598 | 56.429 | 30.022 | 1.00 | 40.00 | 6 |
| | ATOM | 1431 | CD | GLU | A | 445 | 14.875 | 56.472 | 29.239 | 1.00 | 40.00 | 6 |
| | ATOM | 1432 | OE1 | GLU | A | 445 | 15.155 | 55.565 | 28.414 | 1.00 | 40.00 | 8 |
| 15 | ATOM | 1433 | OE2 | GLU | A | 445 | 15.663 | 57.430 | 29.430 | 1.00 | 40.00 | 8 |
| | ATOM | 1434 | C | GLU | A | 445 | 10.724 | 53.912 | 30.049 | 1.00 | 71.46 | 6 |
| | ATOM | 1435 | O | GLU | A | 445 | 10.536 | 53.701 | 28.844 | 1.00 | 73.02 | 8 |
| | ATOM | 1436 | N | CYS | A | 446 | 10.301 | 53.099 | 30.999 | 1.00 | 71.12 | 7 |
| | ATOM | 1437 | CA | CYS | A | 446 | 9.628 | 51.899 | 30.634 | 1.00 | 70.83 | 6 |
| 20 | ATOM | 1438 | CB | CYS | A | 446 | 10.595 | 50.719 | 30.687 | 1.00 | 71.05 | 6 |
| | ATOM | 1439 | SG | CYS | A | 446 | 12.009 | 50.842 | 29.573 | 1.00 | 72.83 | 16 |
| | ATOM | 1440 | C | CYS | A | 446 | 8.454 | 51.671 | 31.535 | 1.00 | 71.91 | 6 |
| | ATOM | 1441 | O | CYS | A | 446 | 8.495 | 52.014 | 32.728 | 1.00 | 72.06 | 8 |
| | ATOM | 1442 | N | PRO | A | 447 | 7.372 | 51.133 | 30.978 | 1.00 | 73.12 | 7 |
| 25 | ATOM | 1443 | CD | PRO | A | 447 | 7.267 | 50.764 | 29.560 | 1.00 | 72.88 | 6 |
| | ATOM | 1444 | CA | PRO | A | 447 | 6.150 | 50.853 | 31.740 | 1.00 | 74.22 | 6 |
| | ATOM | 1445 | CB | PRO | A | 447 | 5.187 | 50.281 | 30.714 | 1.00 | 72.98 | 6 |
| | ATOM | 1446 | CG | PRO | A | 447 | 5.875 | 50.271 | 29.437 | 1.00 | 74.77 | 6 |
| | ATOM | 1447 | C | PRO | A | 447 | 6.435 | 49.843 | 32.831 | 1.00 | 75.94 | 6 |
| 30 | ATOM | 1448 | O | PRO | A | 447 | 7.181 | 48.908 | 32.612 | 1.00 | 76.67 | 8 |
| | ATOM | 1449 | N | THR | A | 448 | 5.820 | 50.002 | 33.997 | 1.00 | 76.91 | 7 |
| | ATOM | 1450 | CA | THR | A | 448 | 6.024 | 49.066 | 35.113 | 1.00 | 78.24 | 6 |
| | ATOM | 1451 | CB | THR | A | 448 | 5.528 | 49.734 | 36.401 | 1.00 | 81.33 | 6 |
| | ATOM | 1452 | OG1 | THR | A | 448 | 4.105 | 49.917 | 36.328 | 1.00 | 84.46 | 8 |
| 35 | ATOM | 1453 | CG2 | THR | A | 448 | 6.192 | 51.081 | 36.585 | 1.00 | 83.51 | 6 |
| | ATOM | 1454 | C | THR | A | 448 | 5.113 | 47.912 | 34.755 | 1.00 | 77.42 | 6 |
| | ATOM | 1455 | O | THR | A | 448 | 4.915 | 46.995 | 35.519 | 1.00 | 77.65 | 8 |
| | ATOM | 1456 | N | GLU | A | 449 | 4.539 | 48.021 | 33.565 | 1.00 | 76.29 | 7 |
| | ATOM | 1457 | CA | GLU | A | 449 | 3.630 | 47.023 | 33.024 | 1.00 | 75.03 | 6 |
| 40 | ATOM | 1458 | CB | GLU | A | 449 | 2.600 | 47.773 | 32.191 | 1.00 | 74.62 | 6 |
| | ATOM | 1459 | CG | GLU | A | 449 | 2.145 | 47.051 | 31.001 | 1.00 | 40.00 | 6 |
| | ATOM | 1460 | CD | GLU | A | 449 | 1.297 | 47.889 | 30.178 | 1.00 | 40.00 | 6 |
| | ATOM | 1461 | OE1 | GLU | A | 449 | 1.479 | 49.137 | 30.146 | 1.00 | 40.00 | 8 |
| | ATOM | 1462 | OE2 | GLU | A | 449 | 0.424 | 47.322 | 29.497 | 1.00 | 40.00 | 8 |
| 45 | ATOM | 1463 | C | GLU | A | 449 | 4.434 | 46.036 | 32.179 | 1.00 | 73.49 | 6 |
| | ATOM | 1464 | O | GLU | A | 449 | 3.882 | 45.142 | 31.559 | 1.00 | 70.24 | 8 |
| | ATOM | 1465 | N | LEU | A | 450 | 5.747 | 46.224 | 32.161 | 1.00 | 70.80 | 7 |
| | ATOM | 1466 | CA | LEU | A | 450 | 6.608 | 45.347 | 31.378 | 1.00 | 68.82 | 6 |
| | ATOM | 1467 | CB | LEU | A | 450 | 7.301 | 46.154 | 30.277 | 1.00 | 71.91 | 6 |
| 50 | ATOM | 1468 | CG | LEU | A | 450 | 6.464 | 46.819 | 29.217 | 1.00 | 76.62 | 6 |
| | ATOM | 1469 | CD1 | LEU | A | 450 | 7.337 | 47.662 | 28.328 | 1.00 | 77.95 | 6 |
| | ATOM | 1470 | CD2 | LEU | A | 450 | 5.786 | 45.750 | 28.415 | 1.00 | 76.46 | 6 |
| | ATOM | 1471 | C | LEU | A | 450 | 7.669 | 44.673 | 32.243 | 1.00 | 66.22 | 6 |
| | ATOM | 1472 | O | LEU | A | 450 | 8.427 | 43.841 | 31.752 | 1.00 | 66.01 | 8 |
| 55 | ATOM | 1473 | N | PHE | A | 451 | 7.705 | 45.039 | 33.530 | 1.00 | 61.96 | 7 |
| | ATOM | 1474 | CA | PHE | A | 451 | 8.681 | 44.506 | 34.480 | 1.00 | 58.44 | 6 |
| | ATOM | 1475 | CB | PHE | A | 451 | 9.041 | 45.562 | 35.540 | 1.00 | 61.34 | 6 |
| | ATOM | 1476 | CG | PHE | A | 451 | 9.873 | 46.717 | 35.008 | 1.00 | 63.02 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 1477 | CD1 | PHE | A | 451 | 9.426 | 47.507 | 33.963 | 1.00 | 62.92 | 6 |
| | ATOM | 1478 | CD2 | PHE | A | 451 | 11.089 | 47.017 | 35.593 | 1.00 | 63.07 | 6 |
| | ATOM | 1479 | CE1 | PHE | A | 451 | 10.199 | 48.598 | 33.521 | 1.00 | 65.12 | 6 |
| | ATOM | 1480 | CE2 | PHE | A | 451 | 11.860 | 48.102 | 35.156 | 1.00 | 64.66 | 6 |
| | ATOM | 1481 | CZ | PHE | A | 451 | 11.410 | 48.897 | 34.118 | 1.00 | 67.12 | 6 |
| 10 | ATOM | 1482 | C | PHE | A | 451 | 8.259 | 43.264 | 35.260 | 1.00 | 56.41 | 6 |
| | ATOM | 1483 | O | PHE | A | 451 | 7.641 | 43.392 | 36.331 | 1.00 | 56.56 | 8 |
| | ATOM | 1484 | N | PRO | A | 452 | 8.555 | 42.045 | 34.755 | 1.00 | 53.28 | 7 |
| | ATOM | 1485 | CD | PRO | A | 452 | 9.177 | 41.689 | 33.481 | 1.00 | 50.46 | 6 |
| | ATOM | 1486 | CA | PRO | A | 452 | 8.153 | 40.859 | 35.543 | 1.00 | 50.26 | 6 |
| 15 | ATOM | 1487 | CB | PRO | A | 452 | 8.739 | 39.680 | 34.780 | 1.00 | 49.19 | 6 |
| | ATOM | 1488 | CG | PRO | A | 452 | 9.178 | 40.206 | 33.482 | 1.00 | 45.89 | 6 |
| | ATOM | 1489 | C | PRO | A | 452 | 8.770 | 40.999 | 36.935 | 1.00 | 49.62 | 6 |
| | ATOM | 1490 | O | PRO | A | 452 | 9.867 | 41.529 | 37.094 | 1.00 | 52.35 | 8 |
| | ATOM | 1491 | N | PRO | A | 453 | 8.139 | 40.425 | 37.947 | 1.00 | 51.50 | 7 |
| 20 | ATOM | 1492 | CD | PRO | A | 453 | 7.001 | 39.542 | 37.797 | 1.00 | 49.66 | 6 |
| | ATOM | 1493 | CA | PRO | A | 453 | 8.610 | 40.528 | 39.323 | 1.00 | 50.89 | 6 |
| | ATOM | 1494 | CB | PRO | A | 453 | 7.675 | 39.659 | 40.109 | 1.00 | 51.49 | 6 |
| | ATOM | 1495 | CG | PRO | A | 453 | 6.703 | 39.141 | 39.185 | 1.00 | 50.82 | 6 |
| | ATOM | 1496 | C | PRO | A | 453 | 10.015 | 40.084 | 39.532 | 1.00 | 50.99 | 6 |
| 25 | ATOM | 1497 | O | PRO | A | 453 | 10.876 | 40.900 | 39.838 | 1.00 | 54.17 | 8 |
| | ATOM | 1498 | N | LEU | A | 454 | 10.255 | 38.781 | 39.423 | 1.00 | 51.21 | 7 |
| | ATOM | 1499 | CA | LEU | A | 454 | 11.585 | 38.298 | 39.674 | 1.00 | 47.17 | 6 |
| | ATOM | 1500 | CB | LEU | A | 454 | 11.813 | 36.962 | 38.975 | 1.00 | 44.44 | 6 |
| | ATOM | 1501 | CG | LEU | A | 454 | 13.167 | 36.375 | 39.289 | 1.00 | 41.33 | 6 |
| 30 | ATOM | 1502 | CD1 | LEU | A | 454 | 13.524 | 36.638 | 40.720 | 1.00 | 35.93 | 6 |
| | ATOM | 1503 | CD2 | LEU | A | 454 | 13.169 | 34.907 | 38.992 | 1.00 | 34.79 | 6 |
| | ATOM | 1504 | C | LEU | A | 454 | 12.541 | 39.375 | 39.182 | 1.00 | 42.25 | 6 |
| | ATOM | 1505 | O | LEU | A | 454 | 13.477 | 39.718 | 39.886 | 1.00 | 40.82 | 8 |
| | ATOM | 1506 | N | PHE | A | 455 | 12.270 | 39.957 | 38.011 | 1.00 | 39.29 | 7 |
| 35 | ATOM | 1507 | CA | PHE | A | 455 | 13.133 | 41.005 | 37.473 | 1.00 | 41.81 | 6 |
| | ATOM | 1508 | CB | PHE | A | 455 | 12.527 | 41.592 | 36.192 | 1.00 | 47.22 | 6 |
| | ATOM | 1509 | CG | PHE | A | 455 | 13.433 | 42.565 | 35.467 | 1.00 | 56.97 | 6 |
| | ATOM | 1510 | CD1 | PHE | A | 455 | 14.715 | 42.189 | 35.135 | 1.00 | 57.23 | 6 |
| | ATOM | 1511 | CD2 | PHE | A | 455 | 12.999 | 43.840 | 35.126 | 1.00 | 59.40 | 6 |
| 40 | ATOM | 1512 | CE1 | PHE | A | 455 | 15.557 | 43.059 | 34.466 | 1.00 | 56.58 | 6 |
| | ATOM | 1513 | CE2 | PHE | A | 455 | 13.848 | 44.716 | 34.452 | 1.00 | 61.80 | 6 |
| | ATOM | 1514 | CZ | PHE | A | 455 | 15.129 | 44.322 | 34.126 | 1.00 | 59.94 | 6 |
| | ATOM | 1515 | C | PHE | A | 455 | 13.273 | 42.085 | 38.534 | 1.00 | 45.12 | 6 |
| | ATOM | 1516 | O | PHE | A | 455 | 14.361 | 42.323 | 39.034 | 1.00 | 39.95 | 8 |
| 45 | ATOM | 1517 | N | LEU | A | 456 | 12.155 | 42.735 | 38.849 | 1.00 | 43.92 | 7 |
| | ATOM | 1518 | CA | LEU | A | 456 | 12.122 | 43.803 | 39.840 | 1.00 | 44.08 | 6 |
| | ATOM | 1519 | CB | LEU | A | 456 | 10.680 | 44.251 | 40.093 | 1.00 | 50.20 | 6 |
| | ATOM | 1520 | CG | LEU | A | 456 | 10.062 | 45.242 | 39.144 | 1.00 | 55.79 | 6 |
| | ATOM | 1521 | CD1 | LEU | A | 456 | 8.598 | 45.432 | 39.450 | 1.00 | 54.70 | 6 |
| 50 | ATOM | 1522 | CD2 | LEU | A | 456 | 10.807 | 46.548 | 39.295 | 1.00 | 53.01 | 6 |
| | ATOM | 1523 | C | LEU | A | 456 | 12.739 | 43.355 | 41.136 | 1.00 | 44.65 | 6 |
| | ATOM | 1524 | O | LEU | A | 456 | 13.597 | 44.022 | 41.685 | 1.00 | 45.93 | 8 |
| | ATOM | 1525 | N | GLU | A | 457 | 11.973 | 41.761 | 41.851 | 1.00 | 44.56 | 7 |
| | ATOM | 1526 | CA | GLU | A | 457 | 12.475 | 41.179 | 43.105 | 1.00 | 46.37 | 6 |
| 55 | ATOM | 1527 | C | GLU | A | 457 | 14.005 | 41.236 | 43.132 | 1.00 | 43.60 | 6 |
| | ATOM | 1528 | O | GLU | A | 457 | 14.583 | 41.724 | 44.117 | 1.00 | 42.69 | 8 |
| | ATOM | 1529 | CB | GLU | A | 457 | 12.024 | 39.723 | 43.223 | 1.00 | 50.16 | 6 |
| | ATOM | 1530 | CG | GLU | A | 457 | 11.114 | 39.476 | 44.427 | 1.00 | 20.00 | 6 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 1531 | CD | GLU | A | 457 | 10.807 | 37.994 | 44.648 | 1.00 | 20.00 | 6 |
| | ATOM | 1532 | OE1 | GLU | A | 457 | 11.673 | 37.099 | 44.311 | 1.00 | 20.00 | 8 |
| | ATOM | 1533 | OE2 | GLU | A | 457 | 9.683 | 37.639 | 45.172 | 1.00 | 20.00 | 8 |
| | ATOM | 1534 | N | VAL | A | 458 | 14.928 | 41.078 | 41.903 | 1.00 | 43.21 | 7 |
| | ATOM | 1535 | CA | VAL | A | 458 | 16.412 | 41.094 | 41.868 | 1.00 | 44.98 | 6 |
| 10 | ATOM | 1536 | CB | VAL | A | 458 | 16.881 | 40.306 | 40.642 | 1.00 | 44.83 | 6 |
| | ATOM | 1537 | CG1 | VAL | A | 458 | 18.365 | 40.106 | 40.698 | 1.00 | 49.72 | 6 |
| | ATOM | 1538 | CG2 | VAL | A | 458 | 16.185 | 38.979 | 40.558 | 1.00 | 40.89 | 6 |
| | ATOM | 1539 | C | VAL | A | 458 | 17.130 | 42.420 | 41.877 | 1.00 | 42.72 | 6 |
| | ATOM | 1540 | O | VAL | A | 458 | 18.061 | 42.617 | 42.658 | 1.00 | 42.88 | 8 |
| 15 | ATOM | 1541 | N | PHE | A | 459 | 16.713 | 43.325 | 41.010 | 1.00 | 44.53 | 7 |
| | ATOM | 1542 | CA | PHE | A | 459 | 17.385 | 44.606 | 40.892 | 1.00 | 48.18 | 6 |
| | ATOM | 1543 | CB | PHE | A | 459 | 17.281 | 45.104 | 39.494 | 1.00 | 43.60 | 6 |
| | ATOM | 1544 | CG | PHE | A | 459 | 17.915 | 44.190 | 38.547 | 1.00 | 40.79 | 6 |
| | ATOM | 1545 | CD1 | PHE | A | 459 | 17.325 | 42.983 | 38.244 | 1.00 | 41.01 | 6 |
| 20 | ATOM | 1546 | CD2 | PHE | A | 459 | 19.153 | 44.483 | 38.054 | 1.00 | 39.48 | 6 |
| | ATOM | 1547 | CE1 | PHE | A | 459 | 17.988 | 42.081 | 37.441 | 1.00 | 40.62 | 6 |
| | ATOM | 1548 | CE2 | PHE | A | 459 | 19.814 | 43.589 | 37.257 | 1.00 | 36.87 | 6 |
| | ATOM | 1549 | CZ | PHE | A | 459 | 19.233 | 42.385 | 36.940 | 1.00 | 36.39 | 6 |
| | ATOM | 1550 | C | PHE | A | 459 | 16.837 | 45.648 | 41.744 | 1.00 | 52.71 | 6 |
| 25 | ATOM | 1551 | O | PHE | A | 459 | 17.492 | 46.682 | 42.017 | 1.00 | 51.34 | 8 |
| | ATOM | 1552 | N | GLU | A | 460 | 15.606 | 45.422 | 42.161 | 1.00 | 62.92 | 7 |
| | ATOM | 1553 | CA | GLU | A | 460 | 15.066 | 46.428 | 42.965 | 1.00 | 69.33 | 6 |
| | ATOM | 1554 | CB | GLU | A | 460 | 13.552 | 46.352 | 43.094 | 1.00 | 72.95 | 6 |
| | ATOM | 1555 | CG | GLU | A | 460 | 12.978 | 47.767 | 42.957 | 1.00 | 78.35 | 6 |
| 30 | ATOM | 1556 | CD | GLU | A | 460 | 12.246 | 48.261 | 44.157 | 1.00 | 82.97 | 6 |
| | ATOM | 1557 | OE1 | GLU | A | 460 | 12.471 | 47.759 | 45.281 | 1.00 | 88.28 | 8 |
| | ATOM | 1558 | OE2 | GLU | A | 460 | 11.422 | 49.200 | 44.017 | 1.00 | 84.80 | 8 |
| | ATOM | 1559 | C | GLU | A | 460 | 15.736 | 46.245 | 44.272 | 1.00 | 71.87 | 6 |
| | ATOM | 1560 | O | GLU | A | 460 | 16.187 | 45.170 | 44.691 | 1.00 | 74.51 | 8 |
| 35 | ATOM | 1561 | N | ASP | A | 461 | 15.790 | 47.373 | 44.917 | 1.00 | 78.50 | 7 |
| | ATOM | 1562 | CA | ASP | A | 461 | 16.415 | 47.505 | 46.173 | 1.00 | 84.19 | 6 |
| | ATOM | 1563 | CB | ASP | A | 461 | 16.394 | 48.981 | 46.471 | 1.00 | 85.82 | 6 |
| | ATOM | 1564 | CG | ASP | A | 461 | 16.801 | 49.786 | 45.276 | 1.00 | 89.62 | 6 |
| | ATOM | 1565 | OD1 | ASP | A | 461 | 16.692 | 49.344 | 44.086 | 1.00 | 93.00 | 8 |
| 40 | ATOM | 1566 | OD2 | ASP | A | 461 | 17.239 | 50.923 | 45.482 | 1.00 | 93.04 | 8 |
| | ATOM | 1567 | C | ASP | A | 461 | 15.639 | 46.703 | 47.214 | 1.00 | 86.80 | 6 |
| | ATOM | 1568 | O | ASP | A | 461 | 16.245 | 45.748 | 47.731 | 1.00 | 88.70 | 8 |
| | ATOM | 1569 | OXT | ASP | A | 461 | 14.457 | 47.026 | 47.451 | 1.00 | 88.70 | 8 |
| | TER | | | | | | | | | | | |
| 45 | ATOM | 1 | CB | LYS | B | 211 | -20.802 | 66.251 | 39.780 | 1.00 | 46.72 | 6 |
| | ATOM | 2 | CG | LYS | B | 211 | -19.566 | 65.345 | 39.922 | 1.00 | 56.48 | 6 |
| | ATOM | 3 | CD | LYS | B | 211 | -18.264 | 66.114 | 40.045 | 1.00 | 60.93 | 6 |
| | ATOM | 4 | CE | LYS | B | 211 | -18.043 | 67.067 | 38.886 | 1.00 | 61.95 | 6 |
| | ATOM | 5 | NZ | LYS | B | 211 | -19.008 | 68.224 | 38.903 | 1.00 | 69.93 | 7 |
| 50 | ATOM | 6 | C | LYS | B | 211 | -22.418 | 67.861 | 40.818 | 1.00 | 35.68 | 6 |
| | ATOM | 7 | O | LYS | B | 211 | -23.356 | 67.113 | 40.454 | 1.00 | 33.58 | 8 |
| | ATOM | 8 | N | LYS | B | 211 | -20.742 | 66.675 | 42.239 | 1.00 | 45.76 | 7 |
| | ATOM | 9 | CA | LYS | B | 211 | -20.998 | 67.285 | 40.894 | 1.00 | 43.42 | 6 |
| | ATOM | 10 | N | PRO | B | 212 | -22.610 | 69.205 | 41.068 | 1.00 | 35.64 | 7 |
| 55 | ATOM | 11 | CD | PRO | B | 212 | -21.526 | 70.177 | 41.287 | 1.00 | 38.60 | 6 |
| | ATOM | 12 | CA | PRO | B | 212 | -23.943 | 69.861 | 41.036 | 1.00 | 38.35 | 6 |
| | ATOM | 13 | CB | PRO | B | 212 | -23.657 | 71.320 | 41.420 | 1.00 | 38.95 | 6 |
| | ATOM | 14 | CG | PRO | B | 212 | -22.226 | 71.474 | 41.551 | 1.00 | 42.00 | 6 |

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|----|------|----|-----|-----------|---------|--------|--------|------|-------|---|
| 5 | ATOM | 15 | C | PRO B 212 | -24.798 | 69.772 | 39.807 | 1.00 | 38.78 | 6 |
| | ATOM | 16 | O | PRO B 212 | -24.350 | 70.045 | 38.696 | 1.00 | 34.64 | 8 |
| | ATOM | 17 | N | GLU B 213 | -26.058 | 69.424 | 40.032 | 1.00 | 40.31 | 7 |
| | ATOM | 18 | CA | GLU B 213 | -27.081 | 69.290 | 39.003 | 1.00 | 43.87 | 6 |
| | ATOM | 19 | CB | GLU B 213 | -27.895 | 68.004 | 39.265 | 1.00 | 45.16 | 6 |
| 10 | ATOM | 20 | CG | GLU B 213 | -27.032 | 66.709 | 39.286 | 1.00 | 47.60 | 6 |
| | ATOM | 21 | CD | GLU B 213 | -27.807 | 65.421 | 39.199 | 1.00 | 50.68 | 6 |
| | ATOM | 22 | OE1 | GLU B 213 | -28.847 | 65.244 | 39.886 | 1.00 | 59.18 | 8 |
| | ATOM | 23 | OE2 | GLU B 213 | -27.382 | 64.516 | 38.442 | 1.00 | 49.06 | 8 |
| | ATOM | 24 | C | GLU B 213 | -27.924 | 70.576 | 39.080 | 1.00 | 45.96 | 6 |
| 15 | ATOM | 25 | O | GLU B 213 | -27.624 | 71.467 | 39.859 | 1.00 | 43.13 | 8 |
| | ATOM | 26 | N | PRO B 214 | -28.987 | 70.698 | 38.308 | 1.00 | 46.52 | 7 |
| | ATOM | 27 | CD | PRO B 214 | -29.484 | 69.635 | 37.446 | 1.00 | 46.44 | 6 |
| | ATOM | 28 | CA | PRO B 214 | -29.843 | 71.907 | 38.302 | 1.00 | 47.52 | 6 |
| | ATOM | 29 | CB | PRO B 214 | -30.799 | 71.639 | 37.210 | 1.00 | 45.40 | 6 |
| 20 | ATOM | 30 | CG | PRO B 214 | -30.530 | 70.257 | 36.805 | 1.00 | 49.89 | 6 |
| | ATOM | 31 | C | PRO B 214 | -30.574 | 72.330 | 39.535 | 1.00 | 45.70 | 6 |
| | ATOM | 32 | O | PRO B 214 | -30.597 | 71.595 | 40.483 | 1.00 | 44.49 | 8 |
| | ATOM | 33 | N | THR B 215 | -31.180 | 73.515 | 39.506 | 1.00 | 45.24 | 7 |
| | ATOM | 34 | CA | THR B 215 | -31.965 | 74.036 | 40.652 | 1.00 | 49.36 | 6 |
| 25 | ATOM | 35 | CB | THR B 215 | -31.443 | 75.420 | 41.091 | 1.00 | 44.86 | 6 |
| | ATOM | 36 | OG1 | THR B 215 | -32.249 | 76.464 | 40.534 | 1.00 | 52.26 | 8 |
| | ATOM | 37 | CG2 | THR B 215 | -30.011 | 75.617 | 40.659 | 1.00 | 39.43 | 6 |
| | ATOM | 38 | C | THR B 215 | -33.386 | 74.239 | 40.114 | 1.00 | 52.51 | 6 |
| | ATOM | 39 | O | THR B 215 | -33.562 | 74.868 | 39.078 | 1.00 | 53.48 | 8 |
| 30 | ATOM | 40 | N | ASP B 216 | -34.387 | 73.741 | 40.829 | 1.00 | 58.81 | 7 |
| | ATOM | 41 | CA | ASP B 216 | -35.795 | 73.865 | 40.435 | 1.00 | 61.51 | 6 |
| | ATOM | 42 | CB | ASP B 216 | -36.674 | 74.005 | 41.650 | 1.00 | 70.57 | 6 |
| | ATOM | 43 | CG | ASP B 216 | -37.675 | 72.981 | 41.710 | 1.00 | 78.07 | 6 |
| | ATOM | 44 | OD1 | ASP B 216 | -38.228 | 72.588 | 40.652 | 1.00 | 82.31 | 8 |
| 35 | ATOM | 45 | OD2 | ASP B 216 | -37.983 | 72.567 | 42.830 | 1.00 | 86.55 | 8 |
| | ATOM | 46 | C | ASP B 216 | -35.920 | 75.123 | 39.648 | 1.00 | 58.42 | 6 |
| | ATOM | 47 | O | ASP B 216 | -36.847 | 75.317 | 38.827 | 1.00 | 56.85 | 8 |
| | ATOM | 48 | N | GLU B 217 | -34.954 | 75.979 | 39.984 | 1.00 | 54.92 | 7 |
| | ATOM | 49 | CA | GLU B 217 | -34.851 | 77.259 | 39.353 | 1.00 | 53.37 | 6 |
| 40 | ATOM | 50 | CB | GLU B 217 | -34.104 | 78.264 | 40.251 | 1.00 | 51.02 | 6 |
| | ATOM | 51 | CG | GLU B 217 | -34.151 | 79.689 | 39.679 | 1.00 | 40.00 | 6 |
| | ATOM | 52 | CD | GLU B 217 | -34.301 | 80.745 | 40.739 | 1.00 | 40.00 | 6 |
| | ATOM | 53 | OE1 | GLU B 217 | -34.089 | 80.443 | 41.945 | 1.00 | 40.00 | 8 |
| | ATOM | 54 | OE2 | GLU B 217 | -34.625 | 81.921 | 40.411 | 1.00 | 40.00 | 8 |
| 45 | ATOM | 55 | C | GLU B 217 | -34.232 | 77.163 | 37.957 | 1.00 | 53.55 | 6 |
| | ATOM | 56 | O | GLU B 217 | -34.815 | 77.612 | 37.018 | 1.00 | 54.33 | 8 |
| | ATOM | 57 | N | GLU B 218 | -33.063 | 76.572 | 37.839 | 1.00 | 49.20 | 7 |
| | ATOM | 58 | CA | GLU B 218 | -32.318 | 76.385 | 36.608 | 1.00 | 45.94 | 6 |
| | ATOM | 59 | CB | GLU B 218 | -30.965 | 75.793 | 36.981 | 1.00 | 43.43 | 6 |
| 50 | ATOM | 60 | CG | GLU B 218 | -30.065 | 76.728 | 37.801 | 1.00 | 40.86 | 6 |
| | ATOM | 61 | CD | GLU B 218 | -28.713 | 76.159 | 38.072 | 1.00 | 39.88 | 6 |
| | ATOM | 62 | OE1 | GLU B 218 | -28.606 | 74.967 | 38.449 | 1.00 | 37.61 | 8 |
| | ATOM | 63 | OE2 | GLU B 218 | -27.707 | 76.901 | 37.945 | 1.00 | 34.01 | 8 |
| | ATOM | 64 | C | GLU B 218 | -33.014 | 75.475 | 35.610 | 1.00 | 44.71 | 6 |
| 55 | ATOM | 65 | O | GLU B 218 | -32.935 | 75.686 | 34.405 | 1.00 | 45.31 | 8 |
| | ATOM | 66 | N | TRP B 219 | -33.669 | 74.439 | 36.131 | 1.00 | 44.02 | 7 |
| | ATOM | 67 | CA | TRP B 219 | -34.368 | 73.490 | 35.290 | 1.00 | 46.97 | 6 |
| | ATOM | 68 | CB | TRP B 219 | -35.046 | 72.408 | 36.119 | 1.00 | 48.42 | 6 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 69 | CG | TRP | B | 219 | -34.195 | 71.230 | 36.374 | 1.00 | 54.61 | 6 |
| | ATOM | 70 | CD2 | TRP | B | 219 | -34.048 | 70.120 | 35.478 | 1.00 | 55.24 | 6 |
| | ATOM | 71 | CE2 | TRP | B | 219 | -33.076 | 69.248 | 36.063 | 1.00 | 53.67 | 6 |
| | ATOM | 72 | CE3 | TRP | B | 219 | -34.615 | 69.771 | 34.252 | 1.00 | 54.55 | 6 |
| | ATOM | 73 | CD1 | TRP | B | 219 | -33.399 | 71.019 | 37.415 | 1.00 | 55.75 | 6 |
| 10 | ATOM | 74 | NE1 | TRP | B | 219 | -32.697 | 69.838 | 37.236 | 1.00 | 54.43 | 7 |
| | ATOM | 75 | CZ2 | TRP | B | 219 | -32.635 | 68.075 | 35.431 | 1.00 | 52.54 | 6 |
| | ATOM | 76 | CZ3 | TRP | B | 219 | -34.214 | 68.603 | 33.643 | 1.00 | 55.17 | 6 |
| | ATOM | 77 | CH2 | TRP | B | 219 | -33.234 | 67.758 | 34.214 | 1.00 | 55.59 | 6 |
| | ATOM | 78 | C | TRP | B | 219 | -35.409 | 74.199 | 34.459 | 1.00 | 47.32 | 6 |
| 15 | ATOM | 79 | O | TRP | B | 219 | -35.561 | 73.914 | 33.277 | 1.00 | 43.56 | 8 |
| | ATOM | 80 | N | GLU | B | 220 | -36.126 | 75.130 | 35.084 | 1.00 | 49.91 | 7 |
| | ATOM | 81 | CA | GLU | B | 220 | -37.158 | 75.874 | 34.402 | 1.00 | 53.57 | 6 |
| | ATOM | 82 | CB | GLU | B | 220 | -37.811 | 76.820 | 35.373 | 1.00 | 58.18 | 6 |
| | ATOM | 83 | CG | GLU | B | 220 | -39.251 | 76.812 | 35.221 | 1.00 | 73.13 | 6 |
| 20 | ATOM | 84 | CD | GLU | B | 220 | -39.824 | 76.858 | 36.489 | 1.00 | 80.06 | 6 |
| | ATOM | 85 | OE1 | GLU | B | 220 | -39.485 | 75.995 | 37.324 | 1.00 | 82.12 | 8 |
| | ATOM | 86 | OE2 | GLU | B | 220 | -40.635 | 77.740 | 36.718 | 1.00 | 82.78 | 8 |
| | ATOM | 87 | C | GLU | B | 220 | -36.539 | 76.645 | 33.250 | 1.00 | 50.51 | 6 |
| | ATOM | 88 | O | GLU | B | 220 | -37.160 | 76.793 | 32.195 | 1.00 | 49.94 | 8 |
| 25 | ATOM | 89 | N | LEU | B | 221 | -35.312 | 77.135 | 33.455 | 1.00 | 43.71 | 7 |
| | ATOM | 90 | CA | LEU | B | 221 | -34.604 | 77.884 | 32.411 | 1.00 | 42.81 | 6 |
| | ATOM | 91 | CB | LEU | B | 221 | -33.214 | 78.324 | 32.865 | 1.00 | 39.21 | 6 |
| | ATOM | 92 | CG | LEU | B | 221 | -32.321 | 78.833 | 31.754 | 1.00 | 36.34 | 6 |
| | ATOM | 93 | CD1 | LEU | B | 221 | -33.073 | 79.843 | 30.927 | 1.00 | 36.93 | 6 |
| 30 | ATOM | 94 | CD2 | LEU | B | 221 | -31.058 | 79.446 | 32.331 | 1.00 | 24.18 | 6 |
| | ATOM | 95 | C | LEU | B | 221 | -34.454 | 77.011 | 31.192 | 1.00 | 43.46 | 6 |
| | ATOM | 96 | O | LEU | B | 221 | -34.819 | 77.406 | 30.104 | 1.00 | 45.25 | 8 |
| | ATOM | 97 | N | ILE | B | 222 | -33.878 | 75.829 | 31.398 | 1.00 | 39.09 | 7 |
| | ATOM | 98 | CA | ILE | B | 222 | -33.687 | 74.857 | 30.330 | 1.00 | 35.47 | 6 |
| 35 | ATOM | 99 | CB | ILE | B | 222 | -33.224 | 73.516 | 30.871 | 1.00 | 33.74 | 6 |
| | ATOM | 100 | CG2 | ILE | B | 222 | -33.204 | 72.488 | 29.776 | 1.00 | 28.86 | 6 |
| | ATOM | 101 | CG1 | ILE | B | 222 | -31.840 | 73.631 | 31.493 | 1.00 | 33.33 | 6 |
| | ATOM | 102 | CD1 | ILE | B | 222 | -31.435 | 72.419 | 32.264 | 1.00 | 34.85 | 6 |
| | ATOM | 103 | C | ILE | B | 222 | -34.991 | 74.627 | 29.598 | 1.00 | 34.26 | 6 |
| 40 | ATOM | 104 | O | ILE | B | 222 | -35.082 | 74.832 | 28.392 | 1.00 | 31.90 | 8 |
| | ATOM | 105 | N | LYS | B | 223 | -35.992 | 74.183 | 30.346 | 1.00 | 39.49 | 7 |
| | ATOM | 106 | CA | LYS | B | 223 | -37.300 | 73.892 | 29.785 | 1.00 | 44.43 | 6 |
| | ATOM | 107 | CB | LYS | B | 223 | -38.351 | 73.876 | 30.882 | 1.00 | 50.81 | 6 |
| | ATOM | 108 | CG | LYS | B | 223 | -39.693 | 73.358 | 30.411 | 1.00 | 62.51 | 6 |
| 45 | ATOM | 109 | CD | LYS | B | 223 | -40.795 | 73.532 | 31.449 | 1.00 | 72.22 | 6 |
| | ATOM | 110 | CE | LYS | B | 223 | -42.163 | 73.249 | 30.827 | 1.00 | 74.55 | 6 |
| | ATOM | 111 | NZ | LYS | B | 223 | -43.268 | 73.378 | 31.837 | 1.00 | 75.78 | 7 |
| | ATOM | 112 | C | LYS | B | 223 | -37.648 | 74.942 | 28.755 | 1.00 | 42.81 | 6 |
| | ATOM | 113 | O | LYS | B | 223 | -38.337 | 74.661 | 27.796 | 1.00 | 40.36 | 8 |
| 50 | ATOM | 114 | N | THR | B | 224 | -37.146 | 76.156 | 28.979 | 1.00 | 39.89 | 7 |
| | ATOM | 115 | CA | THR | B | 224 | -37.353 | 77.293 | 28.074 | 1.00 | 39.93 | 6 |
| | ATOM | 116 | CB | THR | B | 224 | -36.956 | 78.609 | 28.776 | 1.00 | 40.57 | 6 |
| | ATOM | 117 | OG1 | THR | B | 224 | -37.646 | 78.740 | 30.028 | 1.00 | 39.27 | 8 |
| | ATOM | 118 | CG2 | THR | B | 224 | -37.273 | 79.805 | 27.893 | 1.00 | 38.11 | 6 |
| 55 | ATOM | 119 | C | THR | B | 224 | -36.521 | 77.094 | 26.789 | 1.00 | 39.96 | 6 |
| | ATOM | 120 | O | THR | B | 224 | -37.043 | 76.677 | 25.756 | 1.00 | 36.67 | 8 |
| | ATOM | 121 | N | VAL | B | 225 | -35.231 | 77.421 | 26.888 | 1.00 | 38.02 | 7 |
| | ATOM | 122 | CA | VAL | B | 225 | -34.263 | 77.295 | 25.801 | 1.00 | 38.12 | 6 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 123 | CB | VAL | B | 225 | -32.869 | 77.015 | 26.348 | 1.00 | 38.19 | 6 |
| | ATOM | 124 | CG1 | VAL | B | 225 | -31.863 | 76.983 | 25.226 | 1.00 | 36.77 | 6 |
| | ATOM | 125 | CG2 | VAL | B | 225 | -32.483 | 78.050 | 27.353 | 1.00 | 41.76 | 6 |
| | ATOM | 126 | C | VAL | B | 225 | -34.656 | 76.191 | 24.843 | 1.00 | 37.52 | 6 |
| | ATOM | 127 | O | VAL | B | 225 | -34.621 | 76.364 | 23.638 | 1.00 | 36.77 | 8 |
| 10 | ATOM | 128 | N | THR | B | 226 | -35.005 | 75.046 | 25.410 | 1.00 | 34.02 | 7 |
| | ATOM | 129 | CA | THR | B | 226 | -35.423 | 73.887 | 24.638 | 1.00 | 34.67 | 6 |
| | ATOM | 130 | CB | THR | B | 226 | -35.677 | 72.707 | 25.574 | 1.00 | 30.56 | 6 |
| | ATOM | 131 | OG1 | THR | B | 226 | -34.432 | 72.225 | 26.084 | 1.00 | 32.20 | 8 |
| | ATOM | 132 | CG2 | THR | B | 226 | -36.413 | 71.595 | 24.874 | 1.00 | 20.99 | 6 |
| 15 | ATOM | 133 | C | THR | B | 226 | -36.664 | 74.170 | 23.803 | 1.00 | 36.41 | 6 |
| | ATOM | 134 | O | THR | B | 226 | -36.633 | 74.054 | 22.578 | 1.00 | 39.64 | 8 |
| | ATOM | 135 | N | ALA | B | 227 | -37.746 | 74.542 | 24.480 | 1.00 | 39.20 | 7 |
| | ATOM | 136 | CA | ALA | B | 227 | -39.008 | 74.861 | 23.822 | 1.00 | 36.93 | 6 |
| | ATOM | 137 | CB | ALA | B | 227 | -39.914 | 75.631 | 24.785 | 1.00 | 38.06 | 6 |
| 20 | ATOM | 138 | C | ALA | B | 227 | -38.686 | 75.719 | 22.608 | 1.00 | 37.69 | 6 |
| | ATOM | 139 | O | ALA | B | 227 | -39.317 | 75.616 | 21.566 | 1.00 | 40.94 | 8 |
| | ATOM | 140 | N | ALA | B | 228 | -37.677 | 76.572 | 22.785 | 1.00 | 32.86 | 7 |
| | ATOM | 141 | CA | ALA | B | 228 | -37.216 | 77.483 | 21.753 | 1.00 | 32.48 | 6 |
| | ATOM | 142 | CB | ALA | B | 228 | -36.252 | 78.458 | 22.358 | 1.00 | 28.25 | 6 |
| 25 | ATOM | 143 | C | ALA | B | 228 | -36.545 | 76.704 | 20.638 | 1.00 | 36.12 | 6 |
| | ATOM | 144 | O | ALA | B | 228 | -37.078 | 76.586 | 19.544 | 1.00 | 37.86 | 8 |
| | ATOM | 145 | N | HIS | B | 229 | -35.364 | 76.175 | 20.924 | 1.00 | 33.58 | 7 |
| | ATOM | 146 | CA | HIS | B | 229 | -34.611 | 75.409 | 19.956 | 1.00 | 32.97 | 6 |
| | ATOM | 147 | CB | HIS | B | 229 | -33.418 | 74.721 | 20.597 | 1.00 | 33.69 | 6 |
| 30 | ATOM | 148 | CG | HIS | B | 229 | -32.776 | 73.714 | 19.715 | 1.00 | 28.39 | 6 |
| | ATOM | 149 | CD2 | HIS | B | 229 | -32.535 | 72.384 | 19.863 | 1.00 | 28.83 | 6 |
| | ATOM | 150 | ND1 | HIS | B | 229 | -32.336 | 74.030 | 18.426 | 1.00 | 30.47 | 7 |
| | ATOM | 151 | CE1 | HIS | B | 229 | -31.867 | 72.929 | 17.855 | 1.00 | 26.95 | 6 |
| | ATOM | 152 | NE2 | HIS | B | 229 | -31.976 | 71.927 | 18.700 | 1.00 | 31.27 | 7 |
| 35 | ATOM | 153 | C | HIS | B | 229 | -35.362 | 74.352 | 19.202 | 1.00 | 38.40 | 6 |
| | ATOM | 154 | O | HIS | B | 229 | -35.069 | 74.131 | 18.045 | 1.00 | 41.49 | 8 |
| | ATOM | 155 | N | VAL | B | 230 | -36.296 | 73.688 | 19.882 | 1.00 | 38.55 | 7 |
| | ATOM | 156 | CA | VAL | B | 230 | -37.077 | 72.634 | 19.263 | 1.00 | 40.40 | 6 |
| | ATOM | 157 | CB | VAL | B | 230 | -37.744 | 71.747 | 20.310 | 1.00 | 44.68 | 6 |
| 40 | ATOM | 158 | CG1 | VAL | B | 230 | -38.381 | 70.537 | 19.637 | 1.00 | 39.39 | 6 |
| | ATOM | 159 | CG2 | VAL | B | 230 | -36.742 | 71.311 | 21.356 | 1.00 | 42.18 | 6 |
| | ATOM | 160 | C | VAL | B | 230 | -38.133 | 73.130 | 18.284 | 1.00 | 44.28 | 6 |
| | ATOM | 161 | O | VAL | B | 230 | -38.375 | 72.505 | 17.248 | 1.00 | 45.94 | 8 |
| | ATOM | 162 | N | ALA | B | 231 | -38.774 | 74.240 | 18.623 | 1.00 | 45.59 | 7 |
| 45 | ATOM | 163 | CA | ALA | B | 231 | -39.820 | 74.804 | 17.792 | 1.00 | 47.84 | 6 |
| | ATOM | 164 | CB | ALA | B | 231 | -40.736 | 75.661 | 18.647 | 1.00 | 45.08 | 6 |
| | ATOM | 165 | C | ALA | B | 231 | -39.235 | 75.636 | 16.673 | 1.00 | 48.04 | 6 |
| | ATOM | 166 | O | ALA | B | 231 | -39.959 | 76.128 | 15.816 | 1.00 | 49.95 | 8 |
| | ATOM | 167 | N | THR | B | 232 | -37.914 | 75.773 | 16.669 | 1.00 | 47.26 | 7 |
| 50 | ATOM | 168 | CA | THR | B | 232 | -37.220 | 76.563 | 15.654 | 1.00 | 43.64 | 6 |
| | ATOM | 169 | CB | THR | B | 232 | -36.482 | 77.746 | 16.315 | 1.00 | 41.93 | 6 |
| | ATOM | 170 | OG1 | THR | B | 232 | -35.385 | 77.270 | 17.098 | 1.00 | 39.10 | 8 |
| | ATOM | 171 | CG2 | THR | B | 232 | -37.423 | 78.523 | 17.232 | 1.00 | 29.80 | 6 |
| | ATOM | 172 | C | THR | B | 232 | -36.194 | 75.719 | 14.914 | 1.00 | 43.97 | 6 |
| 55 | ATOM | 173 | O | THR | B | 232 | -35.401 | 76.252 | 14.155 | 1.00 | 40.55 | 8 |
| | ATOM | 174 | N | ASN | B | 233 | -36.195 | 74.407 | 15.157 | 1.00 | 48.62 | 7 |
| | ATOM | 175 | CA | ASN | B | 233 | -35.247 | 73.511 | 14.483 | 1.00 | 58.62 | 6 |
| | ATOM | 176 | CB | ASN | B | 233 | -34.621 | 72.537 | 15.500 | 1.00 | 62.44 | 6 |

| | | | | | | | | | | | | |
|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 177 | CG | ASN | B | 233 | -33.407 | 71.812 | 14.946 | 1.00 | 68.35 | 6 |
| | ATOM | 178 | OD1 | ASN | B | 233 | -32.569 | 72.427 | 14.256 | 1.00 | 65.50 | 8 |
| | ATOM | 179 | ND2 | ASN | B | 233 | -33.288 | 70.529 | 15.265 | 1.00 | 74.29 | 7 |
| | ATOM | 180 | C | ASN | B | 233 | -36.033 | 72.755 | 13.437 | 1.00 | 65.06 | 6 |
| | ATOM | 181 | O | ASN | B | 233 | -36.950 | 72.005 | 13.754 | 1.00 | 69.47 | 8 |
| 10 | ATOM | 182 | N | ALA | B | 234 | -35.674 | 72.986 | 12.182 | 1.00 | 68.80 | 7 |
| | ATOM | 183 | CA | ALA | B | 234 | -36.352 | 72.376 | 11.036 | 1.00 | 70.98 | 6 |
| | ATOM | 184 | CB | ALA | B | 234 | -35.585 | 72.701 | 9.769 | 1.00 | 71.43 | 6 |
| | ATOM | 185 | C | ALA | B | 234 | -36.556 | 70.880 | 11.111 | 1.00 | 73.83 | 6 |
| | ATOM | 186 | O | ALA | B | 234 | -35.677 | 70.142 | 11.501 | 1.00 | 74.33 | 8 |
| 15 | ATOM | 187 | N | GLN | B | 235 | -37.754 | 70.479 | 10.717 | 1.00 | 75.07 | 7 |
| | ATOM | 188 | CA | GLN | B | 235 | -38.149 | 69.095 | 10.690 | 1.00 | 76.32 | 6 |
| | ATOM | 189 | CB | GLN | B | 235 | -37.468 | 68.365 | 9.533 | 1.00 | 76.98 | 6 |
| | ATOM | 190 | CG | GLN | B | 235 | -38.120 | 68.540 | 8.170 | 1.00 | 77.07 | 6 |
| | ATOM | 191 | CD | GLN | B | 235 | -38.572 | 69.940 | 7.909 | 1.00 | 80.85 | 6 |
| 20 | ATOM | 192 | OE1 | GLN | B | 235 | -39.575 | 70.401 | 8.491 | 1.00 | 82.01 | 8 |
| | ATOM | 193 | NE2 | GLN | B | 235 | -37.862 | 70.620 | 7.040 | 1.00 | 78.80 | 7 |
| | ATOM | 194 | C | GLN | B | 235 | -37.904 | 68.331 | 11.953 | 1.00 | 77.15 | 6 |
| | ATOM | 195 | O | GLN | B | 235 | -38.087 | 67.137 | 11.947 | 1.00 | 76.06 | 8 |
| | ATOM | 196 | N | GLY | B | 236 | -37.511 | 68.985 | 13.039 | 1.00 | 77.46 | 7 |
| 25 | ATOM | 197 | CA | GLY | B | 236 | -37.304 | 68.263 | 14.288 | 1.00 | 78.37 | 6 |
| | ATOM | 198 | C | GLY | B | 236 | -36.717 | 66.882 | 14.217 | 1.00 | 79.43 | 6 |
| | ATOM | 199 | O | GLY | B | 236 | -35.717 | 66.650 | 13.542 | 1.00 | 79.47 | 8 |
| | ATOM | 200 | N | SER | B | 237 | -37.420 | 66.007 | 14.943 | 1.00 | 77.98 | 7 |
| | ATOM | 201 | CA | SER | B | 237 | -37.117 | 64.600 | 15.092 | 1.00 | 76.49 | 6 |
| 30 | ATOM | 202 | CB | SER | B | 237 | -38.118 | 63.953 | 16.066 | 1.00 | 76.46 | 6 |
| | ATOM | 203 | C | SER | B | 237 | -37.181 | 63.895 | 13.737 | 1.00 | 75.35 | 6 |
| | ATOM | 204 | O | SER | B | 237 | -36.493 | 62.911 | 13.524 | 1.00 | 75.47 | 8 |
| | ATOM | 205 | N | HIS | B | 238 | -38.004 | 64.443 | 12.845 | 1.00 | 75.56 | 7 |
| | ATOM | 206 | CA | HIS | B | 238 | -38.293 | 63.926 | 11.519 | 1.00 | 75.46 | 6 |
| 35 | ATOM | 207 | CB | HIS | B | 238 | -39.663 | 64.397 | 11.096 | 1.00 | 75.85 | 6 |
| | ATOM | 208 | C | HIS | B | 238 | -37.369 | 64.216 | 10.380 | 1.00 | 74.10 | 6 |
| | ATOM | 209 | O | HIS | B | 238 | -37.747 | 64.135 | 9.222 | 1.00 | 75.34 | 8 |
| | ATOM | 210 | N | TRP | B | 239 | -36.127 | 64.427 | 10.651 | 1.00 | 73.39 | 7 |
| | ATOM | 211 | CA | TRP | B | 239 | -35.345 | 64.786 | 9.519 | 1.00 | 74.02 | 6 |
| 40 | ATOM | 212 | CB | TRP | B | 239 | -34.121 | 65.542 | 9.934 | 1.00 | 81.77 | 6 |
| | ATOM | 213 | CG | TRP | B | 239 | -33.085 | 64.786 | 10.737 | 1.00 | 89.67 | 6 |
| | ATOM | 214 | CD2 | TRP | B | 239 | -31.727 | 64.530 | 10.302 | 1.00 | 93.19 | 6 |
| | ATOM | 215 | CE2 | TRP | B | 239 | -31.069 | 63.848 | 11.393 | 1.00 | 95.46 | 6 |
| | ATOM | 216 | CE3 | TRP | B | 239 | -30.949 | 64.941 | 9.196 | 1.00 | 95.35 | 6 |
| 45 | ATOM | 217 | CD1 | TRP | B | 239 | -33.237 | 64.180 | 11.926 | 1.00 | 94.16 | 6 |
| | ATOM | 218 | NE1 | TRP | B | 239 | -32.022 | 63.631 | 12.347 | 1.00 | 97.48 | 7 |
| | ATOM | 219 | CZ2 | TRP | B | 239 | -29.706 | 63.475 | 11.348 | 1.00 | 96.23 | 6 |
| | ATOM | 220 | CZ3 | TRP | B | 239 | -29.613 | 64.533 | 9.128 | 1.00 | 96.75 | 6 |
| | ATOM | 221 | CH2 | TRP | B | 239 | -28.978 | 63.870 | 10.215 | 1.00 | 97.32 | 6 |
| 50 | ATOM | 222 | C | TRP | B | 239 | -34.994 | 63.722 | 8.539 | 1.00 | 70.77 | 6 |
| | ATOM | 223 | O | TRP | B | 239 | -35.423 | 63.772 | 7.388 | 1.00 | 71.70 | 8 |
| | ATOM | 224 | N | LYS | B | 240 | -34.165 | 62.791 | 8.955 | 1.00 | 67.10 | 7 |
| | ATOM | 225 | CA | LYS | B | 240 | -33.724 | 61.744 | 8.077 | 1.00 | 65.63 | 6 |
| | ATOM | 226 | CB | LYS | B | 240 | -33.321 | 60.539 | 8.906 | 1.00 | 66.65 | 6 |
| 55 | ATOM | 227 | CG | LYS | B | 240 | -32.210 | 60.824 | 9.905 | 1.00 | 69.83 | 6 |
| | ATOM | 228 | CD | LYS | B | 240 | -31.759 | 59.553 | 10.602 | 1.00 | 71.49 | 6 |
| | ATOM | 229 | CE | LYS | B | 240 | -30.576 | 59.843 | 11.493 | 1.00 | 71.31 | 6 |
| | ATOM | 230 | NZ | LYS | B | 240 | -30.106 | 58.604 | 12.157 | 1.00 | 72.23 | 7 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 231 | C | LYS | B | 240 | -34.719 | 61.331 | 6.996 | 1.00 | 66.19 | 6 |
| | ATOM | 232 | O | LYS | B | 240 | -34.321 | 60.673 | 6.031 | 1.00 | 65.20 | 8 |
| | ATOM | 233 | N | ASN | B | 241 | -35.986 | 61.727 | 7.139 | 1.00 | 66.69 | 7 |
| | ATOM | 234 | CA | ASN | B | 241 | -37.031 | 61.393 | 6.171 | 1.00 | 67.53 | 6 |
| | ATOM | 235 | CB | ASN | B | 241 | -38.240 | 60.846 | 6.915 | 1.00 | 67.98 | 6 |
| 10 | ATOM | 236 | CG | ASN | B | 241 | -37.966 | 59.479 | 7.544 | 1.00 | 70.19 | 6 |
| | ATOM | 237 | OD1 | ASN | B | 241 | -37.561 | 58.526 | 6.845 | 1.00 | 71.37 | 8 |
| | ATOM | 238 | ND2 | ASN | B | 241 | -38.205 | 59.370 | 8.836 | 1.00 | 71.48 | 7 |
| | ATOM | 239 | C | ASN | B | 241 | -37.496 | 62.532 | 5.255 | 1.00 | 66.62 | 6 |
| | ATOM | 240 | O | ASN | B | 241 | -38.504 | 62.395 | 4.578 | 1.00 | 64.76 | 8 |
| 15 | ATOM | 241 | N | LYS | B | 242 | -36.753 | 63.633 | 5.209 | 1.00 | 66.86 | 7 |
| | ATOM | 242 | CA | LYS | B | 242 | -37.096 | 64.772 | 4.362 | 1.00 | 67.46 | 6 |
| | ATOM | 243 | CB | LYS | B | 242 | -37.501 | 65.948 | 5.258 | 1.00 | 67.93 | 6 |
| | ATOM | 244 | CG | LYS | B | 242 | -38.746 | 65.684 | 6.076 | 1.00 | 71.52 | 6 |
| | ATOM | 245 | CD | LYS | B | 242 | -40.007 | 65.528 | 5.215 | 1.00 | 74.32 | 6 |
| 20 | ATOM | 246 | CE | LYS | B | 242 | -40.416 | 66.852 | 4.564 | 1.00 | 74.41 | 6 |
| | ATOM | 247 | NZ | LYS | B | 242 | -40.657 | 67.941 | 5.575 | 1.00 | 74.44 | 7 |
| | ATOM | 248 | C | LYS | B | 242 | -35.826 | 65.081 | 3.592 | 1.00 | 66.28 | 6 |
| | ATOM | 249 | O | LYS | B | 242 | -35.814 | 65.799 | 2.601 | 1.00 | 67.61 | 8 |
| | ATOM | 250 | N | ARG | B | 243 | -34.763 | 64.485 | 4.112 | 1.00 | 64.19 | 7 |
| 25 | ATOM | 251 | CA | ARG | B | 243 | -33.410 | 64.577 | 3.591 | 1.00 | 62.43 | 6 |
| | ATOM | 252 | CB | ARG | B | 243 | -32.599 | 63.547 | 4.390 | 1.00 | 60.12 | 6 |
| | ATOM | 253 | CG | ARG | B | 243 | -31.128 | 63.558 | 4.171 | 1.00 | 40.00 | 6 |
| | ATOM | 254 | CD | ARG | B | 243 | -30.335 | 62.888 | 5.319 | 1.00 | 40.00 | 6 |
| | ATOM | 255 | NE | ARG | B | 243 | -30.269 | 61.428 | 5.296 | 1.00 | 40.00 | 7 |
| 30 | ATOM | 256 | CZ | ARG | B | 243 | -29.384 | 60.724 | 6.009 | 1.00 | 40.00 | 6 |
| | ATOM | 257 | NH1 | ARG | B | 243 | -28.510 | 61.357 | 6.798 | 1.00 | 40.00 | 7 |
| | ATOM | 258 | NH2 | ARG | B | 243 | -29.355 | 59.401 | 5.908 | 1.00 | 40.00 | 7 |
| | ATOM | 259 | C | ARG | B | 243 | -33.408 | 64.252 | 2.100 | 1.00 | 62.97 | 6 |
| | ATOM | 260 | O | ARG | B | 243 | -33.690 | 63.122 | 1.722 | 1.00 | 63.96 | 8 |
| 35 | ATOM | 261 | N | LYS | B | 244 | -33.105 | 65.245 | 1.270 | 1.00 | 62.41 | 7 |
| | ATOM | 262 | CA | LYS | B | 244 | -33.054 | 65.053 | -0.179 | 1.00 | 61.57 | 6 |
| | ATOM | 263 | CB | LYS | B | 244 | -34.104 | 65.941 | -0.866 | 1.00 | 63.68 | 6 |
| | ATOM | 264 | CG | LYS | B | 244 | -35.527 | 65.731 | -0.337 | 1.00 | 71.29 | 6 |
| | ATOM | 265 | CD | LYS | B | 244 | -36.566 | 66.549 | -1.107 | 1.00 | 73.83 | 6 |
| 40 | ATOM | 266 | CE | LYS | B | 244 | -36.219 | 68.045 | -1.138 | 1.00 | 74.71 | 6 |
| | ATOM | 267 | NZ | LYS | B | 244 | -36.169 | 68.689 | 0.219 | 1.00 | 73.32 | 7 |
| | ATOM | 268 | C | LYS | B | 244 | -31.658 | 65.402 | -0.670 | 1.00 | 59.30 | 6 |
| | ATOM | 269 | O | LYS | B | 244 | -31.317 | 66.570 | -0.852 | 1.00 | 56.34 | 8 |
| | ATOM | 270 | N | PHE | B | 245 | -30.858 | 64.359 | -0.875 | 1.00 | 57.06 | 7 |
| 45 | ATOM | 271 | CA | PHE | B | 245 | -29.462 | 64.525 | -1.305 | 1.00 | 59.01 | 6 |
| | ATOM | 272 | CB | PHE | B | 245 | -28.786 | 63.179 | -1.478 | 1.00 | 59.62 | 6 |
| | ATOM | 273 | CG | PHE | B | 245 | -28.991 | 62.288 | -0.339 | 1.00 | 66.60 | 6 |
| | ATOM | 274 | CD1 | PHE | B | 245 | -30.200 | 61.669 | -0.172 | 1.00 | 67.17 | 6 |
| | ATOM | 275 | CD2 | PHE | B | 245 | -28.012 | 62.117 | 0.593 | 1.00 | 69.25 | 6 |
| 50 | ATOM | 276 | CE1 | PHE | B | 245 | -30.404 | 60.882 | 0.911 | 1.00 | 69.92 | 6 |
| | ATOM | 277 | CE2 | PHE | B | 245 | -28.229 | 61.329 | 1.669 | 1.00 | 70.50 | 6 |
| | ATOM | 278 | CZ | PHE | B | 245 | -29.418 | 60.714 | 1.830 | 1.00 | 70.89 | 6 |
| | ATOM | 279 | C | PHE | B | 245 | -29.301 | 65.282 | -2.592 | 1.00 | 60.68 | 6 |
| | ATOM | 280 | O | PHE | B | 245 | -29.859 | 64.911 | -3.619 | 1.00 | 62.37 | 8 |
| 55 | ATOM | 281 | N | LEU | B | 246 | -28.495 | 66.336 | -2.505 | 1.00 | 60.10 | 7 |
| | ATOM | 282 | CA | LEU | B | 246 | -28.201 | 67.199 | -3.631 | 1.00 | 59.44 | 6 |
| | ATOM | 283 | CB | LEU | B | 246 | -27.248 | 68.332 | -3.231 | 1.00 | 57.43 | 6 |
| | ATOM | 284 | CG | LEU | B | 246 | -27.118 | 69.474 | -4.207 | 1.00 | 54.41 | 6 |

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|----|------|-----|-----|-----|---|-----|---------|--------|---------|------|-------|---|
| 5 | ATOM | 285 | CD1 | LEU | B | 246 | -28.481 | 70.137 | -4.349 | 1.00 | 52.43 | 6 |
| | ATOM | 286 | CD2 | LEU | B | 246 | -26.112 | 70.470 | -3.719 | 1.00 | 51.69 | 6 |
| | ATOM | 287 | C | LEU | B | 246 | -27.585 | 66.379 | -4.740 | 1.00 | 62.05 | 6 |
| | ATOM | 288 | O | LEU | B | 246 | -26.789 | 65.446 | -4.486 | 1.00 | 59.85 | 8 |
| | ATOM | 289 | N | PRO | B | 247 | -27.930 | 66.693 | -5.984 | 1.00 | 63.33 | 7 |
| 10 | ATOM | 290 | CD | PRO | B | 247 | -28.839 | 67.781 | -6.363 | 1.00 | 64.44 | 6 |
| | ATOM | 291 | CA | PRO | B | 247 | -27.391 | 65.958 | -7.130 | 1.00 | 63.56 | 6 |
| | ATOM | 292 | CB | PRO | B | 247 | -27.976 | 66.675 | -8.340 | 1.00 | 64.42 | 6 |
| | ATOM | 293 | CG | PRO | B | 247 | -28.873 | 67.714 | -7.841 | 1.00 | 64.90 | 6 |
| | ATOM | 294 | C | PRO | B | 247 | -25.866 | 65.947 | -7.143 | 1.00 | 61.94 | 6 |
| 15 | ATOM | 295 | O | PRO | B | 247 | -25.223 | 66.944 | -6.856 | 1.00 | 61.60 | 8 |
| | ATOM | 296 | N | GLU | B | 248 | -25.333 | 64.771 | -7.478 | 1.00 | 61.33 | 7 |
| | ATOM | 297 | CA | GLU | B | 248 | -23.896 | 64.516 | -7.590 | 1.00 | 63.50 | 6 |
| | ATOM | 298 | CB | GLU | B | 248 | -23.630 | 63.154 | -8.248 | 1.00 | 66.94 | 6 |
| | ATOM | 299 | CG | GLU | B | 248 | -22.168 | 62.953 | -8.713 | 1.00 | 68.70 | 6 |
| 20 | ATOM | 300 | CD | GLU | B | 248 | -21.898 | 61.745 | -9.580 | 1.00 | 40.00 | 6 |
| | ATOM | 301 | OE1 | GLU | B | 248 | -22.863 | 61.007 | -10.035 | 1.00 | 40.00 | 8 |
| | ATOM | 302 | OE2 | GLU | B | 248 | -20.709 | 61.460 | -9.838 | 1.00 | 40.00 | 8 |
| | ATOM | 303 | C | GLU | B | 248 | -23.158 | 65.571 | -8.415 | 1.00 | 64.19 | 6 |
| | ATOM | 304 | O | GLU | B | 248 | -22.056 | 65.975 | -8.066 | 1.00 | 65.56 | 8 |
| 25 | ATOM | 305 | N | ASP | B | 249 | -23.796 | 66.019 | -9.498 | 1.00 | 64.36 | 7 |
| | ATOM | 306 | CA | ASP | B | 249 | -23.254 | 66.994 | -10.436 | 1.00 | 63.33 | 6 |
| | ATOM | 307 | CB | ASP | B | 249 | -24.122 | 67.031 | -11.698 | 1.00 | 62.97 | 6 |
| | ATOM | 308 | CG | ASP | B | 249 | -25.437 | 67.715 | -11.489 | 1.00 | 64.63 | 6 |
| | ATOM | 309 | OD1 | ASP | B | 249 | -26.235 | 67.285 | -10.629 | 1.00 | 64.84 | 8 |
| 30 | ATOM | 310 | OD2 | ASP | B | 249 | -25.726 | 68.718 | -12.189 | 1.00 | 66.52 | 8 |
| | ATOM | 311 | C | ASP | B | 249 | -23.068 | 68.413 | -9.960 | 1.00 | 64.31 | 6 |
| | ATOM | 312 | O | ASP | B | 249 | -22.117 | 69.084 | -10.355 | 1.00 | 64.73 | 8 |
| | ATOM | 313 | N | ILE | B | 250 | -23.987 | 68.892 | -9.136 | 1.00 | 63.09 | 7 |
| | ATOM | 314 | CA | ILE | B | 250 | -23.921 | 70.281 | -8.660 | 1.00 | 64.39 | 6 |
| 35 | ATOM | 315 | CB | ILE | B | 250 | -25.124 | 70.575 | -7.798 | 1.00 | 65.79 | 6 |
| | ATOM | 316 | CG2 | ILE | B | 250 | -25.559 | 72.041 | -7.858 | 1.00 | 64.78 | 6 |
| | ATOM | 317 | CG1 | ILE | B | 250 | -26.348 | 69.752 | -8.206 | 1.00 | 65.28 | 6 |
| | ATOM | 318 | CD1 | ILE | B | 250 | -27.671 | 70.444 | -7.887 | 1.00 | 65.08 | 6 |
| | ATOM | 319 | C | ILE | B | 250 | -22.815 | 70.488 | -7.714 | 1.00 | 65.21 | 6 |
| 40 | ATOM | 320 | O | ILE | B | 250 | -22.754 | 69.847 | -6.656 | 1.00 | 64.05 | 8 |
| | ATOM | 321 | N | GLY | B | 251 | -22.024 | 71.392 | -8.103 | 1.00 | 65.48 | 7 |
| | ATOM | 322 | CA | GLY | B | 251 | -20.873 | 71.721 | -7.342 | 1.00 | 67.32 | 6 |
| | ATOM | 323 | C | GLY | B | 251 | -19.808 | 70.806 | -7.800 | 1.00 | 68.52 | 6 |
| | ATOM | 324 | O | GLY | B | 251 | -19.791 | 70.548 | -9.025 | 1.00 | 65.49 | 8 |
| 45 | ATOM | 325 | N | GLN | B | 252 | -19.074 | 70.440 | -6.799 | 1.00 | 72.26 | 7 |
| | ATOM | 326 | CA | GLN | B | 252 | -17.949 | 69.540 | -6.883 | 1.00 | 74.10 | 6 |
| | ATOM | 327 | CB | GLN | B | 252 | -18.460 | 68.098 | -6.723 | 1.00 | 75.82 | 6 |
| | ATOM | 328 | CG | GLN | B | 252 | -17.367 | 67.088 | -6.356 | 1.00 | 77.81 | 6 |
| | ATOM | 329 | CD | GLN | B | 252 | -17.924 | 65.759 | -5.824 | 1.00 | 79.38 | 6 |
| 50 | ATOM | 330 | OE1 | GLN | B | 252 | -18.615 | 65.042 | -6.549 | 1.00 | 80.55 | 8 |
| | ATOM | 331 | NE2 | GLN | B | 252 | -17.661 | 65.380 | -4.586 | 1.00 | 78.12 | 7 |
| | ATOM | 332 | C | GLN | B | 252 | -17.258 | 69.727 | -8.258 | 1.00 | 77.17 | 6 |
| | ATOM | 333 | O | GLN | B | 252 | -17.977 | 70.009 | -9.227 | 1.00 | 76.50 | 8 |
| | ATOM | 334 | N | ALA | B | 253 | -15.718 | 69.795 | -8.279 | 1.00 | 80.78 | 7 |
| 55 | ATOM | 335 | CA | ALA | B | 253 | -14.615 | 70.766 | -8.544 | 1.00 | 83.70 | 6 |
| | ATOM | 336 | CB | ALA | B | 253 | -13.794 | 70.914 | -7.255 | 1.00 | 83.23 | 6 |
| | ATOM | 337 | C | ALA | B | 253 | -13.605 | 70.732 | -9.731 | 1.00 | 85.59 | 6 |
| | ATOM | 338 | O | ALA | B | 253 | -13.186 | 69.691 | -10.171 | 1.00 | 85.69 | 8 |

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|----|------|-----|-----|-----------|---------|--------|---------|------|-------|---|
| 5 | ATOM | 339 | N | PRO B 254 | -13.223 | 71.944 | -10.246 | 1.00 | 35.05 | 7 |
| | ATOM | 340 | CD | PRO B 254 | -13.798 | 73.217 | -9.752 | 1.00 | 33.97 | 6 |
| | ATOM | 341 | CA | PRO B 254 | -12.266 | 72.177 | -11.351 | 1.00 | 35.89 | 6 |
| | ATOM | 342 | CB | PRO B 254 | -12.275 | 73.710 | -11.596 | 1.00 | 33.94 | 6 |
| | ATOM | 343 | CG | PRO B 254 | -13.222 | 74.277 | -10.688 | 1.00 | 33.31 | 6 |
| 10 | ATOM | 344 | C | PRO B 254 | -10.827 | 71.665 | -11.121 | 1.00 | 37.75 | 6 |
| | ATOM | 345 | O | PRO B 254 | -10.379 | 71.426 | -10.009 | 1.00 | 38.78 | 8 |
| | TER | | | | | | | | | |
| | ATOM | 1 | N | GLY B 261 | -8.238 | 79.356 | -2.979 | 1.00 | 40.00 | 7 |
| | ATOM | 2 | CA | GLY B 261 | -9.314 | 78.411 | -3.005 | 1.00 | 40.00 | 6 |
| 15 | ATOM | 3 | C | GLY B 261 | -10.206 | 78.717 | -4.355 | 1.00 | 40.00 | 6 |
| | ATOM | 4 | O | GLY B 261 | -11.372 | 79.141 | -4.256 | 1.00 | 40.00 | 8 |
| | ATOM | 5 | N | GLY B 262 | -9.565 | 78.527 | -5.597 | 1.00 | 40.00 | 7 |
| | ATOM | 6 | CA | GLY B 262 | -10.136 | 78.609 | -7.087 | 1.00 | 40.00 | 6 |
| | ATOM | 7 | C | GLY B 262 | -10.849 | 79.966 | -7.577 | 1.00 | 40.00 | 6 |
| 20 | ATOM | 8 | O | GLY B 262 | -10.200 | 81.044 | -7.543 | 1.00 | 40.00 | 8 |
| | ATOM | 9 | N | LYS B 263 | -12.086 | 79.687 | -8.124 | 1.00 | 61.71 | 7 |
| | ATOM | 10 | CA | LYS B 263 | -13.323 | 80.536 | -8.428 | 1.00 | 64.36 | 6 |
| | ATOM | 11 | C | LYS B 263 | -14.367 | 79.750 | -7.614 | 1.00 | 63.41 | 6 |
| | ATOM | 12 | O | LYS B 263 | -14.102 | 78.579 | -7.280 | 1.00 | 61.93 | 8 |
| 25 | ATOM | 13 | CB | LYS B 263 | -13.901 | 80.405 | -9.876 | 1.00 | 63.50 | 6 |
| | ATOM | 14 | CG | LYS B 263 | -13.487 | 81.474 | -10.881 | 1.00 | 20.00 | 6 |
| | ATOM | 15 | CD | LYS B 263 | -14.016 | 82.897 | -10.612 | 1.00 | 20.00 | 6 |
| | ATOM | 16 | CE | LYS B 263 | -13.641 | 83.874 | -11.742 | 1.00 | 20.00 | 6 |
| | ATOM | 17 | NZ | LYS B 263 | -13.680 | 85.287 | -11.341 | 1.00 | 20.00 | 7 |
| 30 | ATOM | 18 | N | VAL B 264 | -15.489 | 80.335 | -7.307 | 1.00 | 61.15 | 7 |
| | ATOM | 19 | CA | VAL B 264 | -16.616 | 79.632 | -6.619 | 1.00 | 59.46 | 6 |
| | ATOM | 20 | CB | VAL B 264 | -17.574 | 80.703 | -6.099 | 1.00 | 59.03 | 6 |
| | ATOM | 21 | CG1 | VAL B 264 | -18.479 | 80.215 | -4.979 | 1.00 | 53.79 | 6 |
| | ATOM | 22 | CG2 | VAL B 264 | -16.847 | 81.938 | -5.562 | 1.00 | 55.32 | 6 |
| 35 | ATOM | 23 | C | VAL B 264 | -17.330 | 78.824 | -7.700 | 1.00 | 60.96 | 6 |
| | ATOM | 24 | O | VAL B 264 | -16.940 | 78.873 | -8.873 | 1.00 | 62.13 | 8 |
| | ATOM | 25 | N | ASP B 265 | -18.378 | 78.098 | -7.340 | 1.00 | 62.59 | 7 |
| | ATOM | 26 | CA | ASP B 265 | -19.175 | 77.339 | -8.312 | 1.00 | 64.95 | 6 |
| | ATOM | 27 | CB | ASP B 265 | -18.796 | 75.851 | -8.270 | 1.00 | 64.32 | 6 |
| 40 | ATOM | 28 | CG | ASP B 265 | -19.928 | 75.022 | -8.584 | 1.00 | 67.70 | 6 |
| | ATOM | 29 | OD1 | ASP B 265 | -20.856 | 75.062 | -9.295 | 1.00 | 72.59 | 8 |
| | ATOM | 30 | OD2 | ASP B 265 | -20.370 | 73.959 | -8.310 | 1.00 | 68.84 | 8 |
| | ATOM | 31 | C | ASP B 265 | -20.658 | 77.614 | -8.016 | 1.00 | 65.64 | 6 |
| | ATOM | 32 | O | ASP B 265 | -21.342 | 76.895 | -7.313 | 1.00 | 68.81 | 8 |
| 45 | ATOM | 33 | N | LEU B 266 | -21.066 | 78.737 | -8.588 | 1.00 | 65.12 | 7 |
| | ATOM | 34 | CA | LEU B 266 | -22.385 | 79.330 | -8.499 | 1.00 | 63.40 | 6 |
| | ATOM | 35 | CB | LEU B 266 | -22.429 | 80.448 | -9.542 | 1.00 | 67.34 | 6 |
| | ATOM | 36 | CG | LEU B 266 | -21.295 | 81.459 | -9.399 | 1.00 | 69.35 | 6 |
| | ATOM | 37 | CD1 | LEU B 266 | -20.983 | 82.127 | -10.712 | 1.00 | 68.24 | 6 |
| 50 | ATOM | 38 | CD2 | LEU B 266 | -21.663 | 82.461 | -8.344 | 1.00 | 70.47 | 6 |
| | ATOM | 39 | C | LEU B 266 | -23.673 | 78.507 | -8.602 | 1.00 | 59.67 | 6 |
| | ATOM | 40 | O | LEU B 266 | -24.684 | 78.890 | -7.988 | 1.00 | 53.35 | 8 |
| | ATOM | 41 | N | GLU B 267 | -23.677 | 77.416 | -9.371 | 1.00 | 58.01 | 7 |
| | ATOM | 42 | CA | GLU B 267 | -24.901 | 76.640 | -9.449 | 1.00 | 58.34 | 6 |
| 55 | ATOM | 43 | CB | GLU B 267 | -24.752 | 75.410 | -10.368 | 1.00 | 59.21 | 6 |
| | ATOM | 44 | CG | GLU B 267 | -25.979 | 74.464 | -10.268 | 1.00 | 62.89 | 6 |
| | ATOM | 45 | CD | GLU B 267 | -26.048 | 73.419 | -11.328 | 1.00 | 67.66 | 6 |
| | ATOM | 46 | OE1 | GLU B 267 | -25.076 | 72.645 | -11.512 | 1.00 | 69.95 | 8 |

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|----|------|-----|-----|-----|---|-----|---------|--------|---------|------|-------|---|
| 5 | ATOM | 47 | OE2 | GLU | B | 267 | -27.098 | 73.328 | -12.008 | 1.00 | 69.40 | 8 |
| | ATOM | 48 | C | GLU | B | 267 | -25.200 | 76.184 | -8.032 | 1.00 | 57.67 | 6 |
| | ATOM | 49 | O | GLU | B | 267 | -26.354 | 76.009 | -7.643 | 1.00 | 58.34 | 8 |
| | ATOM | 50 | N | ALA | B | 268 | -24.114 | 75.996 | -7.285 | 1.00 | 53.43 | 7 |
| | ATOM | 51 | CA | ALA | B | 268 | -24.151 | 75.560 | -5.905 | 1.00 | 49.00 | 6 |
| 10 | ATOM | 52 | CB | ALA | B | 268 | -22.816 | 74.956 | -5.526 | 1.00 | 45.72 | 6 |
| | ATOM | 53 | C | ALA | B | 268 | -24.421 | 76.775 | -5.056 | 1.00 | 45.76 | 6 |
| | ATOM | 54 | O | ALA | B | 268 | -25.419 | 76.823 | -4.351 | 1.00 | 41.50 | 8 |
| | ATOM | 55 | N | PHE | B | 269 | -23.533 | 77.766 | -5.142 | 1.00 | 41.43 | 7 |
| | ATOM | 56 | CA | PHE | B | 269 | -23.688 | 78.989 | -4.358 | 1.00 | 43.96 | 6 |
| 15 | ATOM | 57 | CB | PHE | B | 269 | -22.903 | 80.150 | -4.971 | 1.00 | 40.10 | 6 |
| | ATOM | 58 | CG | PHE | B | 269 | -23.057 | 81.458 | -4.224 | 1.00 | 40.44 | 6 |
| | ATOM | 59 | CD1 | PHE | B | 269 | -22.284 | 81.727 | -3.105 | 1.00 | 38.98 | 6 |
| | ATOM | 60 | CD2 | PHE | B | 269 | -24.033 | 82.372 | -4.603 | 1.00 | 37.15 | 6 |
| | ATOM | 61 | CE1 | PHE | B | 269 | -22.472 | 82.921 | -2.388 | 1.00 | 32.12 | 6 |
| 20 | ATOM | 62 | CE2 | PHE | B | 269 | -24.228 | 83.567 | -3.890 | 1.00 | 38.41 | 6 |
| | ATOM | 63 | CZ | PHE | B | 269 | -23.457 | 83.838 | -2.780 | 1.00 | 40.55 | 6 |
| | ATOM | 64 | C | PHE | B | 269 | -25.154 | 79.374 | -4.320 | 1.00 | 49.76 | 6 |
| | ATOM | 65 | O | PHE | B | 269 | -25.645 | 79.905 | -3.336 | 1.00 | 52.15 | 8 |
| | ATOM | 66 | N | SER | B | 270 | -25.840 | 79.112 | -5.426 | 1.00 | 53.15 | 7 |
| 25 | ATOM | 67 | CA | SER | B | 270 | -27.253 | 79.431 | -5.520 | 1.00 | 52.29 | 6 |
| | ATOM | 68 | CB | SER | B | 270 | -27.742 | 79.274 | -6.948 | 1.00 | 51.85 | 6 |
| | ATOM | 69 | OG | SER | B | 270 | -29.118 | 79.606 | -7.048 | 1.00 | 53.42 | 8 |
| | ATOM | 70 | C | SER | B | 270 | -28.012 | 78.486 | -4.630 | 1.00 | 49.38 | 6 |
| | ATOM | 71 | O | SER | B | 270 | -28.438 | 78.864 | -3.548 | 1.00 | 48.74 | 8 |
| 30 | ATOM | 72 | N | HIS | B | 271 | -28.185 | 77.253 | -5.115 | 1.00 | 50.15 | 7 |
| | ATOM | 73 | CA | HIS | B | 271 | -28.904 | 76.203 | -4.382 | 1.00 | 51.67 | 6 |
| | ATOM | 74 | CB | HIS | B | 271 | -28.409 | 74.812 | -4.782 | 1.00 | 58.52 | 6 |
| | ATOM | 75 | CG | HIS | B | 271 | -29.096 | 74.248 | -5.976 | 1.00 | 68.97 | 6 |
| | ATOM | 76 | CD2 | HIS | B | 271 | -29.987 | 73.233 | -6.102 | 1.00 | 70.88 | 6 |
| 35 | ATOM | 77 | ND1 | HIS | B | 271 | -28.943 | 74.770 | -7.270 | 1.00 | 71.98 | 7 |
| | ATOM | 78 | CE1 | HIS | B | 271 | -29.716 | 74.080 | -8.100 | 1.00 | 73.91 | 6 |
| | ATOM | 79 | NE2 | HIS | B | 271 | -30.354 | 73.149 | -7.419 | 1.00 | 73.59 | 7 |
| | ATOM | 80 | C | HIS | B | 271 | -28.785 | 76.347 | -2.886 | 1.00 | 48.33 | 6 |
| | ATOM | 81 | O | HIS | B | 271 | -29.641 | 75.874 | -2.156 | 1.00 | 48.39 | 8 |
| 40 | ATOM | 82 | N | PHE | B | 272 | -27.702 | 76.992 | -2.444 | 1.00 | 41.34 | 7 |
| | ATOM | 83 | CA | PHE | B | 272 | -27.440 | 77.224 | -1.033 | 1.00 | 39.44 | 6 |
| | ATOM | 84 | CB | PHE | B | 272 | -25.936 | 77.302 | -0.801 | 1.00 | 36.67 | 6 |
| | ATOM | 85 | CG | PHE | B | 272 | -25.241 | 75.945 | -0.861 | 1.00 | 33.39 | 6 |
| | ATOM | 86 | CD1 | PHE | B | 272 | -23.856 | 75.857 | -0.976 | 1.00 | 33.14 | 6 |
| 45 | ATOM | 87 | CD2 | PHE | B | 272 | -25.973 | 74.767 | -0.732 | 1.00 | 38.28 | 6 |
| | ATOM | 88 | CE1 | PHE | B | 272 | -23.200 | 74.606 | -0.989 | 1.00 | 38.26 | 6 |
| | ATOM | 89 | CE2 | PHE | B | 272 | -25.321 | 73.518 | -0.743 | 1.00 | 43.28 | 6 |
| | ATOM | 90 | CZ | PHE | B | 272 | -23.937 | 73.441 | -0.856 | 1.00 | 39.74 | 6 |
| | ATOM | 91 | C | PHE | B | 272 | -28.144 | 78.472 | -0.477 | 1.00 | 40.75 | 6 |
| 50 | ATOM | 92 | O | PHE | B | 272 | -28.803 | 78.393 | 0.558 | 1.00 | 35.51 | 8 |
| | ATOM | 93 | N | THR | B | 273 | -28.027 | 79.621 | -1.144 | 1.00 | 41.64 | 7 |
| | ATOM | 94 | CA | THR | B | 273 | -28.658 | 80.850 | -0.652 | 1.00 | 45.97 | 6 |
| | ATOM | 95 | CB | THR | B | 273 | -28.023 | 82.105 | -1.283 | 1.00 | 51.52 | 6 |
| | ATOM | 96 | OG1 | THR | B | 273 | -28.292 | 82.151 | -2.688 | 1.00 | 45.74 | 8 |
| 55 | ATOM | 97 | CG2 | THR | B | 273 | -26.511 | 82.123 | -1.048 | 1.00 | 49.73 | 6 |
| | ATOM | 98 | C | THR | B | 273 | -30.142 | 80.859 | -0.971 | 1.00 | 46.23 | 6 |
| | ATOM | 99 | O | THR | B | 273 | -30.862 | 81.751 | -0.535 | 1.00 | 41.21 | 8 |
| | ATOM | 100 | N | LYS | B | 274 | -30.583 | 79.876 | -1.758 | 1.00 | 46.21 | 7 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 101 | CA | LYS | B | 274 | -31.983 | 79.774 | -2.147 | 1.00 | 54.53 | 6 |
| | ATOM | 102 | CB | LYS | B | 274 | -32.133 | 78.724 | -3.232 | 1.00 | 54.36 | 6 |
| | ATOM | 103 | C | LYS | B | 274 | -32.819 | 79.396 | -0.931 | 1.00 | 56.88 | 6 |
| | ATOM | 104 | O | LYS | B | 274 | -34.025 | 79.624 | -0.906 | 1.00 | 57.98 | 8 |
| | ATOM | 105 | N | ILE | B | 275 | -32.151 | 78.820 | 0.076 | 1.00 | 56.48 | 7 |
| 10 | ATOM | 106 | CA | ILE | B | 275 | -32.791 | 78.381 | 1.332 | 1.00 | 52.64 | 6 |
| | ATOM | 107 | CB | ILE | B | 275 | -32.638 | 76.863 | 1.519 | 1.00 | 49.15 | 6 |
| | ATOM | 108 | CG2 | ILE | B | 275 | -33.505 | 76.105 | 0.529 | 1.00 | 47.42 | 6 |
| | ATOM | 109 | CG1 | ILE | B | 275 | -31.188 | 76.441 | 1.343 | 1.00 | 45.31 | 6 |
| | ATOM | 110 | CD1 | ILE | B | 275 | -30.990 | 74.952 | 1.391 | 1.00 | 37.22 | 6 |
| 15 | ATOM | 111 | C | ILE | B | 275 | -32.241 | 79.086 | 2.574 | 1.00 | 51.78 | 6 |
| | ATOM | 112 | O | ILE | B | 275 | -32.858 | 79.049 | 3.622 | 1.00 | 49.80 | 8 |
| | ATOM | 113 | N | ILE | B | 276 | -31.071 | 79.709 | 2.435 | 1.00 | 51.76 | 7 |
| | ATOM | 114 | CA | ILE | B | 276 | -30.410 | 80.409 | 3.533 | 1.00 | 52.58 | 6 |
| | ATOM | 115 | CB | ILE | B | 276 | -29.145 | 81.110 | 3.042 | 1.00 | 55.04 | 6 |
| 20 | ATOM | 116 | CG2 | ILE | B | 276 | -29.486 | 82.172 | 2.017 | 1.00 | 53.28 | 6 |
| | ATOM | 117 | CG1 | ILE | B | 276 | -28.396 | 81.786 | 4.203 | 1.00 | 57.31 | 6 |
| | ATOM | 118 | CD1 | ILE | B | 276 | -27.862 | 80.854 | 5.231 | 1.00 | 60.32 | 6 |
| | ATOM | 119 | C | ILE | B | 276 | -31.282 | 81.461 | 4.237 | 1.00 | 50.70 | 6 |
| | ATOM | 120 | O | ILE | B | 276 | -31.015 | 81.817 | 5.385 | 1.00 | 55.55 | 8 |
| 25 | ATOM | 121 | N | THR | B | 277 | -32.322 | 81.953 | 3.568 | 1.00 | 47.33 | 7 |
| | ATOM | 122 | CA | THR | B | 277 | -33.174 | 82.968 | 4.141 | 1.00 | 42.59 | 6 |
| | ATOM | 123 | CB | THR | B | 277 | -34.042 | 83.632 | 3.048 | 1.00 | 44.97 | 6 |
| | ATOM | 124 | OG1 | THR | B | 277 | -33.202 | 84.145 | 2.001 | 1.00 | 46.38 | 8 |
| | ATOM | 125 | CG2 | THR | B | 277 | -34.856 | 84.781 | 3.653 | 1.00 | 37.17 | 6 |
| 30 | ATOM | 126 | C | THR | B | 277 | -34.069 | 82.447 | 5.267 | 1.00 | 39.84 | 6 |
| | ATOM | 127 | O | THR | B | 277 | -34.083 | 83.026 | 6.375 | 1.00 | 40.55 | 8 |
| | ATOM | 128 | N | PRO | B | 278 | -34.832 | 81.385 | 5.017 | 1.00 | 38.20 | 7 |
| | ATOM | 129 | CD | PRO | B | 278 | -34.925 | 80.666 | 3.747 | 1.00 | 36.34 | 6 |
| | ATOM | 130 | CA | PRO | B | 278 | -35.711 | 80.834 | 6.059 | 1.00 | 36.63 | 6 |
| 35 | ATOM | 131 | CB | PRO | B | 278 | -36.475 | 79.715 | 5.357 | 1.00 | 32.95 | 6 |
| | ATOM | 132 | CG | PRO | B | 278 | -35.833 | 79.516 | 4.056 | 1.00 | 35.75 | 6 |
| | ATOM | 133 | C | PRO | B | 278 | -34.892 | 80.324 | 7.220 | 1.00 | 38.60 | 6 |
| | ATOM | 134 | O | PRO | B | 278 | -35.372 | 80.157 | 8.331 | 1.00 | 37.67 | 8 |
| | ATOM | 135 | N | ALA | B | 279 | -33.636 | 80.040 | 6.927 | 1.00 | 37.05 | 7 |
| 40 | ATOM | 136 | CA | ALA | B | 279 | -32.696 | 79.525 | 7.903 | 1.00 | 33.18 | 6 |
| | ATOM | 137 | CB | ALA | B | 279 | -31.391 | 79.195 | 7.205 | 1.00 | 30.56 | 6 |
| | ATOM | 138 | C | ALA | B | 279 | -32.447 | 80.536 | 8.991 | 1.00 | 33.47 | 6 |
| | ATOM | 139 | O | ALA | B | 279 | -32.623 | 80.238 | 10.158 | 1.00 | 33.74 | 8 |
| | ATOM | 140 | N | ILE | B | 280 | -32.010 | 81.728 | 8.577 | 1.00 | 29.96 | 7 |
| 45 | ATOM | 141 | CA | ILE | B | 280 | -31.728 | 82.809 | 9.501 | 1.00 | 25.94 | 6 |
| | ATOM | 142 | CB | ILE | B | 280 | -31.190 | 84.040 | 8.754 | 1.00 | 26.95 | 6 |
| | ATOM | 143 | CG2 | ILE | B | 280 | -30.881 | 85.149 | 9.715 | 1.00 | 15.40 | 6 |
| | ATOM | 144 | CG1 | ILE | B | 280 | -29.904 | 83.696 | 8.007 | 1.00 | 26.73 | 6 |
| | ATOM | 145 | CD1 | ILE | B | 280 | -29.255 | 84.878 | 7.362 | 1.00 | 34.31 | 6 |
| 50 | ATOM | 146 | C | ILE | B | 280 | -32.964 | 83.172 | 10.310 | 1.00 | 31.39 | 6 |
| | ATOM | 147 | O | ILE | B | 280 | -32.882 | 83.378 | 11.522 | 1.00 | 35.69 | 8 |
| | ATOM | 148 | N | THR | B | 281 | -34.113 | 83.233 | 9.647 | 1.00 | 30.90 | 7 |
| | ATOM | 149 | CA | THR | B | 281 | -35.361 | 83.586 | 10.328 | 1.00 | 33.49 | 6 |
| | ATOM | 150 | CB | THR | B | 281 | -36.598 | 83.396 | 9.419 | 1.00 | 37.18 | 6 |
| 55 | ATOM | 151 | OG1 | THR | B | 281 | -36.703 | 82.034 | 9.005 | 1.00 | 46.48 | 8 |
| | ATOM | 152 | CG2 | THR | B | 281 | -36.525 | 84.289 | 8.198 | 1.00 | 32.85 | 6 |
| | ATOM | 153 | C | THR | B | 281 | -35.523 | 82.706 | 11.556 | 1.00 | 29.94 | 6 |
| | ATOM | 154 | O | THR | B | 281 | -35.855 | 83.186 | 12.634 | 1.00 | 25.55 | 8 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 155 | N | ARG | B | 282 | -35.296 | 81.405 | 11.378 | 1.00 | 32.70 | 7 |
| | ATOM | 156 | CA | ARG | B | 282 | -35.439 | 80.449 | 12.475 | 1.00 | 34.27 | 6 |
| | ATOM | 157 | CB | ARG | B | 282 | -34.999 | 79.060 | 12.020 | 1.00 | 33.78 | 6 |
| | ATOM | 158 | CG | ARG | B | 282 | -35.986 | 77.944 | 12.280 | 1.00 | 45.15 | 6 |
| | ATOM | 159 | CD | ARG | B | 282 | -36.701 | 77.514 | 11.015 | 1.00 | 58.24 | 6 |
| 10 | ATOM | 160 | NE | ARG | B | 282 | -35.771 | 77.153 | 9.969 | 1.00 | 68.41 | 7 |
| | ATOM | 161 | CZ | ARG | B | 282 | -34.862 | 76.200 | 10.098 | 1.00 | 72.31 | 6 |
| | ATOM | 162 | NH1 | ARG | B | 282 | -34.779 | 75.502 | 11.232 | 1.00 | 77.89 | 7 |
| | ATOM | 163 | NH2 | ARG | B | 282 | -34.022 | 75.963 | 9.096 | 1.00 | 69.25 | 7 |
| | ATOM | 164 | C | ARG | B | 282 | -34.556 | 80.919 | 13.622 | 1.00 | 34.81 | 6 |
| 15 | ATOM | 165 | O | ARG | B | 282 | -35.008 | 81.034 | 14.753 | 1.00 | 36.03 | 8 |
| | ATOM | 166 | N | VAL | B | 283 | -33.288 | 81.183 | 13.289 | 1.00 | 31.71 | 7 |
| | ATOM | 167 | CA | VAL | B | 283 | -32.304 | 81.667 | 14.249 | 1.00 | 30.16 | 6 |
| | ATOM | 168 | CB | VAL | B | 283 | -30.993 | 82.029 | 13.559 | 1.00 | 29.00 | 6 |
| | ATOM | 169 | CG1 | VAL | B | 283 | -30.015 | 82.617 | 14.557 | 1.00 | 28.64 | 6 |
| 20 | ATOM | 170 | CG2 | VAL | B | 283 | -30.385 | 80.816 | 12.915 | 1.00 | 28.28 | 6 |
| | ATOM | 171 | C | VAL | B | 283 | -32.848 | 82.884 | 14.994 | 1.00 | 32.50 | 6 |
| | ATOM | 172 | O | VAL | B | 283 | -32.619 | 83.057 | 16.185 | 1.00 | 33.48 | 8 |
| | ATOM | 173 | N | VAL | B | 284 | -33.573 | 83.728 | 14.265 | 1.00 | 30.96 | 7 |
| | ATOM | 174 | CA | VAL | B | 284 | -34.177 | 84.925 | 14.844 | 1.00 | 29.14 | 6 |
| 25 | ATOM | 175 | CB | VAL | B | 284 | -34.672 | 85.892 | 13.751 | 1.00 | 31.27 | 6 |
| | ATOM | 176 | CG1 | VAL | B | 284 | -35.278 | 87.129 | 14.371 | 1.00 | 24.21 | 6 |
| | ATOM | 177 | CG2 | VAL | B | 284 | -33.554 | 86.270 | 12.812 | 1.00 | 30.51 | 6 |
| | ATOM | 178 | C | VAL | B | 284 | -35.336 | 84.498 | 15.747 | 1.00 | 28.89 | 6 |
| | ATOM | 179 | O | VAL | B | 284 | -35.491 | 84.994 | 16.860 | 1.00 | 27.29 | 8 |
| 30 | ATOM | 180 | N | ASP | B | 285 | -36.143 | 83.564 | 15.250 | 1.00 | 28.76 | 7 |
| | ATOM | 181 | CA | ASP | B | 285 | -37.299 | 83.057 | 15.983 | 1.00 | 35.32 | 6 |
| | ATOM | 182 | CB | ASP | B | 285 | -38.129 | 82.098 | 15.111 | 1.00 | 33.29 | 6 |
| | ATOM | 183 | CG | ASP | B | 285 | -38.881 | 82.795 | 14.013 | 1.00 | 38.15 | 6 |
| | ATOM | 184 | OD1 | ASP | B | 285 | -39.660 | 83.729 | 14.305 | 1.00 | 34.70 | 8 |
| 35 | ATOM | 185 | OD2 | ASP | B | 285 | -38.741 | 82.406 | 12.821 | 1.00 | 34.43 | 8 |
| | ATOM | 186 | C | ASP | B | 285 | -36.863 | 82.339 | 17.257 | 1.00 | 36.70 | 6 |
| | ATOM | 187 | O | ASP | B | 285 | -37.606 | 82.304 | 18.237 | 1.00 | 37.96 | 8 |
| | ATOM | 188 | N | PHE | B | 286 | -35.663 | 81.755 | 17.235 | 1.00 | 35.96 | 7 |
| | ATOM | 189 | CA | PHE | B | 286 | -35.134 | 81.053 | 18.401 | 1.00 | 37.10 | 6 |
| 40 | ATOM | 190 | CB | PHE | B | 286 | -33.870 | 80.262 | 18.052 | 1.00 | 37.97 | 6 |
| | ATOM | 191 | CG | PHE | B | 286 | -33.079 | 79.818 | 19.258 | 1.00 | 36.50 | 6 |
| | ATOM | 192 | CD1 | PHE | B | 286 | -33.704 | 79.168 | 20.294 | 1.00 | 36.75 | 6 |
| | ATOM | 193 | CD2 | PHE | B | 286 | -31.721 | 80.063 | 19.343 | 1.00 | 33.83 | 6 |
| | ATOM | 194 | CE1 | PHE | B | 286 | -32.987 | 78.769 | 21.401 | 1.00 | 39.55 | 6 |
| 45 | ATOM | 195 | CE2 | PHE | B | 286 | -30.997 | 79.662 | 20.456 | 1.00 | 38.08 | 6 |
| | ATOM | 196 | CZ | PHE | B | 286 | -31.632 | 79.013 | 21.486 | 1.00 | 34.44 | 6 |
| | ATOM | 197 | C | PHE | B | 286 | -34.808 | 82.023 | 19.504 | 1.00 | 36.83 | 6 |
| | ATOM | 198 | O | PHE | B | 286 | -35.246 | 81.845 | 20.631 | 1.00 | 35.61 | 8 |
| | ATOM | 199 | N | ALA | B | 287 | -34.005 | 83.027 | 19.169 | 1.00 | 37.33 | 7 |
| 50 | ATOM | 200 | CA | ALA | B | 287 | -33.599 | 84.035 | 20.132 | 1.00 | 36.34 | 6 |
| | ATOM | 201 | CB | ALA | B | 287 | -32.644 | 85.008 | 19.469 | 1.00 | 36.40 | 6 |
| | ATOM | 202 | C | ALA | B | 287 | -34.831 | 84.769 | 20.657 | 1.00 | 38.76 | 6 |
| | ATOM | 203 | O | ALA | B | 287 | -34.882 | 85.193 | 21.814 | 1.00 | 41.98 | 8 |
| | ATOM | 204 | N | LYS | B | 288 | -35.820 | 84.912 | 19.779 | 1.00 | 38.28 | 7 |
| 55 | ATOM | 205 | CA | LYS | B | 288 | -37.066 | 85.584 | 20.112 | 1.00 | 45.26 | 6 |
| | ATOM | 206 | CB | LYS | B | 288 | -37.983 | 85.690 | 18.898 | 1.00 | 48.35 | 6 |
| | ATOM | 207 | CG | LYS | B | 288 | -37.577 | 86.756 | 17.916 | 1.00 | 51.43 | 6 |
| | ATOM | 208 | CD | LYS | B | 288 | -38.806 | 87.359 | 17.226 | 1.00 | 60.23 | 6 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 209 | CE | LYS | B | 288 | -39.680 | 86.308 | 16.564 | 1.00 | 62.81 | 6 |
| | ATOM | 210 | NZ | LYS | B | 288 | -38.897 | 85.460 | 15.614 | 1.00 | 64.69 | 7 |
| | ATOM | 211 | C | LYS | B | 288 | -37.846 | 84.901 | 21.191 | 1.00 | 43.31 | 6 |
| | ATOM | 212 | O | LYS | B | 288 | -38.650 | 85.532 | 21.857 | 1.00 | 45.66 | 8 |
| | ATOM | 213 | N | LYS | B | 289 | -37.618 | 83.604 | 21.345 | 1.00 | 41.70 | 7 |
| 10 | ATOM | 214 | CA | LYS | B | 289 | -38.313 | 82.849 | 22.351 | 1.00 | 40.67 | 6 |
| | ATOM | 215 | CB | LYS | B | 289 | -38.554 | 81.418 | 21.845 | 1.00 | 42.25 | 6 |
| | ATOM | 216 | CG | LYS | B | 289 | -39.438 | 81.368 | 20.589 | 1.00 | 39.53 | 6 |
| | ATOM | 217 | CD | LYS | B | 289 | -40.093 | 80.010 | 20.422 | 1.00 | 43.19 | 6 |
| | ATOM | 218 | CE | LYS | B | 289 | -41.025 | 79.987 | 19.223 | 1.00 | 45.74 | 6 |
| 15 | ATOM | 219 | NZ | LYS | B | 289 | -42.391 | 80.476 | 19.512 | 1.00 | 52.49 | 7 |
| | ATOM | 220 | C | LYS | B | 289 | -37.555 | 82.871 | 23.668 | 1.00 | 41.50 | 6 |
| | ATOM | 221 | O | LYS | B | 289 | -38.057 | 82.366 | 24.657 | 1.00 | 39.77 | 8 |
| | ATOM | 222 | N | LEU | B | 290 | -36.365 | 83.482 | 23.661 | 1.00 | 40.68 | 7 |
| | ATOM | 223 | CA | LEU | B | 290 | -35.539 | 83.599 | 24.854 | 1.00 | 39.33 | 6 |
| 20 | ATOM | 224 | CB | LEU | B | 290 | -34.053 | 83.499 | 24.491 | 1.00 | 36.14 | 6 |
| | ATOM | 225 | CG | LEU | B | 290 | -33.640 | 82.240 | 23.767 | 1.00 | 34.81 | 6 |
| | ATOM | 226 | CD1 | LEU | B | 290 | -32.147 | 82.255 | 23.523 | 1.00 | 29.07 | 6 |
| | ATOM | 227 | CD2 | LEU | B | 290 | -34.013 | 81.040 | 24.607 | 1.00 | 33.45 | 6 |
| | ATOM | 228 | C | LEU | B | 290 | -35.832 | 84.915 | 25.577 | 1.00 | 40.08 | 6 |
| 25 | ATOM | 229 | O | LEU | B | 290 | -35.479 | 86.006 | 25.088 | 1.00 | 42.00 | 8 |
| | ATOM | 230 | N | PRO | B | 291 | -36.462 | 84.840 | 26.765 | 1.00 | 40.27 | 7 |
| | ATOM | 231 | CD | PRO | B | 291 | -36.819 | 83.613 | 27.494 | 1.00 | 39.65 | 6 |
| | ATOM | 232 | CA | PRO | B | 291 | -36.782 | 86.069 | 27.501 | 1.00 | 38.28 | 6 |
| | ATOM | 233 | CB | PRO | B | 291 | -37.376 | 85.574 | 28.811 | 1.00 | 35.88 | 6 |
| 30 | ATOM | 234 | CG | PRO | B | 291 | -37.549 | 84.110 | 28.695 | 1.00 | 34.19 | 6 |
| | ATOM | 235 | C | PRO | B | 291 | -35.570 | 87.002 | 27.714 | 1.00 | 40.05 | 6 |
| | ATOM | 236 | O | PRO | B | 291 | -35.625 | 88.197 | 27.403 | 1.00 | 41.33 | 8 |
| | ATOM | 237 | N | MET | B | 292 | -34.474 | 86.476 | 28.258 | 1.00 | 40.59 | 7 |
| | ATOM | 238 | CA | MET | B | 292 | -33.296 | 87.286 | 28.545 | 1.00 | 42.86 | 6 |
| 35 | ATOM | 239 | CB | MET | B | 292 | -32.149 | 86.376 | 28.975 | 1.00 | 43.28 | 6 |
| | ATOM | 240 | CG | MET | B | 292 | -32.553 | 85.302 | 29.970 | 1.00 | 50.35 | 6 |
| | ATOM | 241 | SD | MET | B | 292 | -31.070 | 84.609 | 30.755 | 1.00 | 51.17 | 16 |
| | ATOM | 242 | CE | MET | B | 292 | -31.797 | 83.212 | 31.701 | 1.00 | 54.63 | 6 |
| | ATOM | 243 | C | MET | B | 292 | -32.895 | 88.077 | 27.315 | 1.00 | 41.05 | 6 |
| 40 | ATOM | 244 | O | MET | B | 292 | -32.228 | 89.098 | 27.420 | 1.00 | 39.66 | 8 |
| | ATOM | 245 | N | PHE | B | 293 | -33.322 | 87.604 | 26.143 | 1.00 | 39.30 | 7 |
| | ATOM | 246 | CA | PHE | B | 293 | -33.017 | 88.271 | 24.878 | 1.00 | 40.92 | 6 |
| | ATOM | 247 | CB | PHE | B | 293 | -33.296 | 87.329 | 23.707 | 1.00 | 40.98 | 6 |
| | ATOM | 248 | CG | PHE | B | 293 | -32.937 | 87.909 | 22.365 | 1.00 | 42.78 | 6 |
| 45 | ATOM | 249 | CD1 | PHE | B | 293 | -31.653 | 88.354 | 22.120 | 1.00 | 44.40 | 6 |
| | ATOM | 250 | CD2 | PHE | B | 293 | -33.872 | 87.972 | 21.350 | 1.00 | 43.66 | 6 |
| | ATOM | 251 | CE1 | PHE | B | 293 | -31.306 | 88.869 | 20.872 | 1.00 | 39.83 | 6 |
| | ATOM | 252 | CE2 | PHE | B | 293 | -33.525 | 88.486 | 20.100 | 1.00 | 46.21 | 6 |
| | ATOM | 253 | CZ | PHE | B | 293 | -32.239 | 88.926 | 19.859 | 1.00 | 45.18 | 6 |
| 50 | ATOM | 254 | C | PHE | B | 293 | -33.873 | 89.518 | 24.744 | 1.00 | 45.54 | 6 |
| | ATOM | 255 | O | PHE | B | 293 | -33.369 | 90.626 | 24.579 | 1.00 | 42.01 | 8 |
| | ATOM | 256 | N | CYS | B | 294 | -35.181 | 89.305 | 24.808 | 1.00 | 47.05 | 7 |
| | ATOM | 257 | CA | CYS | B | 294 | -36.146 | 90.382 | 24.689 | 1.00 | 50.15 | 6 |
| | ATOM | 258 | CB | CYS | B | 294 | -37.553 | 89.793 | 24.756 | 1.00 | 45.90 | 6 |
| 55 | ATOM | 259 | SG | CYS | B | 294 | -37.899 | 88.607 | 23.449 | 1.00 | 51.50 | 16 |
| | ATOM | 260 | C | CYS | B | 294 | -35.974 | 91.474 | 25.751 | 1.00 | 51.38 | 6 |
| | ATOM | 261 | O | CYS | B | 294 | -36.585 | 92.536 | 25.656 | 1.00 | 53.83 | 8 |
| | ATOM | 262 | N | GLU | B | 295 | -35.137 | 91.200 | 26.753 | 1.00 | 49.72 | 7 |

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|----|------|-----|-----|-----|---|-----|---------|---------|--------|------|-------|----|
| 5 | ATOM | 263 | CA | GLU | B | 295 | -34.839 | 92.159 | 27.816 | 1.00 | 52.53 | 6 |
| | ATOM | 264 | CB | GLU | B | 295 | -34.553 | 91.412 | 29.131 | 1.00 | 57.40 | 6 |
| | ATOM | 265 | CG | GLU | B | 295 | -35.811 | 90.978 | 29.874 | 1.00 | 69.63 | 6 |
| | ATOM | 266 | CD | GLU | B | 295 | -36.610 | 92.144 | 30.375 | 1.00 | 78.49 | 6 |
| | ATOM | 267 | OE1 | GLU | B | 295 | -36.153 | 92.869 | 31.297 | 1.00 | 82.82 | 8 |
| 10 | ATOM | 268 | OE2 | GLU | B | 295 | -37.730 | 92.385 | 29.860 | 1.00 | 85.30 | 8 |
| | ATOM | 269 | C | GLU | B | 295 | -33.629 | 93.009 | 27.415 | 1.00 | 48.54 | 6 |
| | ATOM | 270 | O | GLU | B | 295 | -32.981 | 93.627 | 28.260 | 1.00 | 49.82 | 8 |
| | ATOM | 271 | N | LEU | B | 296 | -33.374 | 93.030 | 26.109 | 1.00 | 43.79 | 7 |
| | ATOM | 272 | CA | LEU | B | 296 | -32.268 | 93.761 | 25.540 | 1.00 | 45.42 | 6 |
| 15 | ATOM | 273 | CB | LEU | B | 296 | -31.319 | 92.769 | 24.838 | 1.00 | 41.04 | 6 |
| | ATOM | 274 | CG | LEU | B | 296 | -30.735 | 91.631 | 25.662 | 1.00 | 42.74 | 6 |
| | ATOM | 275 | CD1 | LEU | B | 296 | -30.354 | 90.478 | 24.764 | 1.00 | 40.99 | 6 |
| | ATOM | 276 | CD2 | LEU | B | 296 | -29.559 | 92.119 | 26.468 | 1.00 | 39.44 | 6 |
| | ATOM | 277 | C | LEU | B | 296 | -32.760 | 94.779 | 24.522 | 1.00 | 45.56 | 6 |
| 20 | ATOM | 278 | O | LEU | B | 296 | -33.845 | 94.600 | 23.924 | 1.00 | 43.07 | 8 |
| | ATOM | 279 | N | PRO | B | 297 | -32.004 | 95.875 | 24.338 | 1.00 | 46.99 | 7 |
| | ATOM | 280 | CD | PRO | B | 297 | -30.740 | 96.123 | 25.046 | 1.00 | 47.12 | 6 |
| | ATOM | 281 | CA | PRO | B | 297 | -32.388 | 96.912 | 23.363 | 1.00 | 49.61 | 6 |
| | ATOM | 282 | CB | PRO | B | 297 | -31.294 | 97.973 | 23.494 | 1.00 | 49.91 | 6 |
| 25 | ATOM | 283 | CG | PRO | B | 297 | -30.302 | 97.477 | 24.545 | 1.00 | 51.28 | 6 |
| | ATOM | 284 | C | PRO | B | 297 | -32.263 | 96.273 | 21.913 | 1.00 | 49.59 | 6 |
| | ATOM | 285 | O | PRO | B | 297 | -31.441 | 95.340 | 21.685 | 1.00 | 51.66 | 8 |
| | ATOM | 286 | N | CYS | B | 298 | -33.035 | 96.667 | 20.854 | 1.00 | 51.02 | 7 |
| | ATOM | 287 | CA | CYS | B | 298 | -32.761 | 96.150 | 19.456 | 1.00 | 52.86 | 6 |
| 30 | ATOM | 288 | CB | CYS | B | 298 | -33.140 | 97.165 | 18.356 | 1.00 | 54.57 | 6 |
| | ATOM | 289 | SG | CYS | B | 298 | -34.884 | 97.085 | 17.836 | 1.00 | 67.87 | 16 |
| | ATOM | 290 | C | CYS | B | 298 | -31.385 | 96.330 | 19.127 | 1.00 | 48.51 | 6 |
| | ATOM | 291 | O | CYS | B | 298 | -30.579 | 95.506 | 18.744 | 1.00 | 49.58 | 8 |
| | ATOM | 292 | N | GLU | B | 299 | -31.107 | 97.447 | 19.230 | 1.00 | 44.17 | 7 |
| 35 | ATOM | 293 | CA | GLU | B | 299 | -29.989 | 97.645 | 18.718 | 1.00 | 47.57 | 6 |
| | ATOM | 294 | CB | GLU | B | 299 | -29.402 | 98.973 | 19.208 | 1.00 | 49.92 | 6 |
| | ATOM | 295 | CG | GLU | B | 299 | -29.944 | 100.187 | 18.433 | 1.00 | 59.30 | 6 |
| | ATOM | 296 | CD | GLU | B | 299 | -31.090 | 100.887 | 19.164 | 1.00 | 63.80 | 6 |
| | ATOM | 297 | OE1 | GLU | B | 299 | -31.673 | 101.904 | 18.629 | 1.00 | 69.03 | 8 |
| 40 | ATOM | 298 | OE2 | GLU | B | 299 | -31.473 | 100.458 | 20.319 | 1.00 | 67.10 | 8 |
| | ATOM | 299 | C | GLU | B | 299 | -28.993 | 96.533 | 18.987 | 1.00 | 46.57 | 6 |
| | ATOM | 300 | O | GLU | B | 299 | -28.200 | 96.179 | 18.111 | 1.00 | 44.65 | 8 |
| | ATOM | 301 | N | ASP | B | 300 | -29.045 | 95.989 | 20.203 | 1.00 | 45.17 | 7 |
| | ATOM | 302 | CA | ASP | B | 300 | -28.152 | 94.908 | 20.584 | 1.00 | 43.32 | 6 |
| 45 | ATOM | 303 | CB | ASP | B | 300 | -27.985 | 94.849 | 22.105 | 1.00 | 37.38 | 6 |
| | ATOM | 304 | CG | ASP | B | 300 | -27.239 | 96.016 | 22.650 | 1.00 | 36.23 | 6 |
| | ATOM | 305 | OD1 | ASP | B | 300 | -26.208 | 96.421 | 22.052 | 1.00 | 35.87 | 8 |
| | ATOM | 306 | OD2 | ASP | B | 300 | -27.661 | 96.543 | 23.716 | 1.00 | 40.14 | 8 |
| | ATOM | 307 | C | ASP | B | 300 | -28.721 | 93.591 | 20.071 | 1.00 | 42.81 | 6 |
| 50 | ATOM | 308 | O | ASP | B | 300 | -28.001 | 92.775 | 19.489 | 1.00 | 46.02 | 8 |
| | ATOM | 309 | N | GLN | B | 301 | -30.019 | 93.399 | 20.306 | 1.00 | 38.60 | 7 |
| | ATOM | 310 | CA | GLN | B | 301 | -30.712 | 92.197 | 19.858 | 1.00 | 40.00 | 6 |
| | ATOM | 311 | CB | GLN | B | 301 | -32.234 | 92.418 | 19.836 | 1.00 | 38.59 | 6 |
| | ATOM | 312 | CG | GLN | B | 301 | -32.908 | 92.380 | 21.187 | 1.00 | 40.26 | 6 |
| 55 | ATOM | 313 | CD | GLN | B | 301 | -34.401 | 92.583 | 21.083 | 1.00 | 44.15 | 6 |
| | ATOM | 314 | OE1 | GLN | B | 301 | -34.859 | 93.637 | 20.589 | 1.00 | 45.73 | 8 |
| | ATOM | 315 | NE2 | GLN | B | 301 | -35.165 | 91.602 | 21.544 | 1.00 | 46.13 | 7 |
| | ATOM | 316 | C | GLN | B | 301 | -30.237 | 91.830 | 18.455 | 1.00 | 41.64 | 6 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 317 | O | GLN | B | 301 | -30.162 | 90.662 | 18.100 | 1.00 | 45.02 | 8 |
| | ATOM | 318 | N | ILE | B | 302 | -29.916 | 92.864 | 17.674 | 1.00 | 41.01 | 7 |
| | ATOM | 319 | CA | ILE | B | 302 | -29.424 | 92.692 | 16.311 | 1.00 | 40.23 | 6 |
| | ATOM | 320 | CB | ILE | B | 302 | -29.584 | 93.978 | 15.498 | 1.00 | 39.52 | 6 |
| | ATOM | 321 | CG2 | ILE | B | 302 | -29.034 | 93.792 | 14.100 | 1.00 | 31.98 | 6 |
| 10 | ATOM | 322 | CG1 | ILE | B | 302 | -31.059 | 94.385 | 15.416 | 1.00 | 40.77 | 6 |
| | ATOM | 323 | CD1 | ILE | B | 302 | -31.939 | 93.317 | 14.775 | 1.00 | 45.43 | 6 |
| | ATOM | 324 | C | ILE | B | 302 | -27.966 | 92.260 | 16.342 | 1.00 | 38.58 | 6 |
| | ATOM | 325 | O | ILE | B | 302 | -27.613 | 91.197 | 15.830 | 1.00 | 40.81 | 8 |
| | ATOM | 326 | N | ILE | B | 303 | -27.128 | 93.111 | 16.933 | 1.00 | 37.50 | 7 |
| 15 | ATOM | 327 | CA | ILE | B | 303 | -25.692 | 92.846 | 17.062 | 1.00 | 39.33 | 6 |
| | ATOM | 328 | CB | ILE | B | 303 | -25.066 | 93.648 | 18.203 | 1.00 | 39.06 | 6 |
| | ATOM | 329 | CG2 | ILE | B | 303 | -23.566 | 93.405 | 18.257 | 1.00 | 36.19 | 6 |
| | ATOM | 330 | CG1 | ILE | B | 303 | -25.309 | 95.143 | 18.020 | 1.00 | 40.15 | 6 |
| | ATOM | 331 | CD1 | ILE | B | 303 | -24.816 | 95.966 | 19.173 | 1.00 | 36.93 | 6 |
| 20 | ATOM | 332 | C | ILE | B | 303 | -25.470 | 91.365 | 17.323 | 1.00 | 36.49 | 6 |
| | ATOM | 333 | O | ILE | B | 303 | -24.619 | 90.725 | 16.712 | 1.00 | 36.58 | 8 |
| | ATOM | 334 | N | LEU | B | 304 | -26.244 | 90.843 | 18.266 | 1.00 | 32.91 | 7 |
| | ATOM | 335 | CA | LEU | B | 304 | -26.194 | 89.433 | 18.633 | 1.00 | 27.55 | 6 |
| | ATOM | 336 | CB | LEU | B | 304 | -27.172 | 89.182 | 19.793 | 1.00 | 22.35 | 6 |
| 25 | ATOM | 337 | CG | LEU | B | 304 | -26.623 | 89.449 | 21.187 | 1.00 | 26.88 | 6 |
| | ATOM | 338 | CD1 | LEU | B | 304 | -25.540 | 90.495 | 21.136 | 1.00 | 24.82 | 6 |
| | ATOM | 339 | CD2 | LEU | B | 304 | -27.747 | 89.840 | 22.121 | 1.00 | 23.69 | 6 |
| | ATOM | 340 | C | LEU | B | 304 | -26.505 | 88.547 | 17.425 | 1.00 | 28.05 | 6 |
| | ATOM | 341 | O | LEU | B | 304 | -25.668 | 87.751 | 16.983 | 1.00 | 24.68 | 8 |
| 30 | ATOM | 342 | N | LEU | B | 305 | -27.716 | 88.700 | 16.897 | 1.00 | 26.34 | 7 |
| | ATOM | 343 | CA | LEU | B | 305 | -28.145 | 87.939 | 15.741 | 1.00 | 30.91 | 6 |
| | ATOM | 344 | CB | LEU | B | 305 | -29.460 | 88.514 | 15.199 | 1.00 | 32.50 | 6 |
| | ATOM | 345 | CG | LEU | B | 305 | -30.699 | 88.305 | 16.050 | 1.00 | 33.36 | 6 |
| | ATOM | 346 | CD1 | LEU | B | 305 | -31.938 | 88.839 | 15.342 | 1.00 | 33.87 | 6 |
| 35 | ATOM | 347 | CD2 | LEU | B | 305 | -30.863 | 86.812 | 16.298 | 1.00 | 31.72 | 6 |
| | ATOM | 348 | C | LEU | B | 305 | -27.072 | 87.922 | 14.666 | 1.00 | 29.76 | 6 |
| | ATOM | 349 | O | LEU | B | 305 | -26.687 | 86.860 | 14.202 | 1.00 | 29.33 | 8 |
| | ATOM | 350 | N | LYS | B | 306 | -26.597 | 89.107 | 14.291 | 1.00 | 29.72 | 7 |
| | ATOM | 351 | CA | LYS | B | 306 | -25.576 | 89.254 | 13.264 | 1.00 | 34.28 | 6 |
| 40 | ATOM | 352 | CB | LYS | B | 306 | -25.224 | 90.732 | 13.077 | 1.00 | 35.98 | 6 |
| | ATOM | 353 | CG | LYS | B | 306 | -26.350 | 91.581 | 12.494 | 1.00 | 43.35 | 6 |
| | ATOM | 354 | CD | LYS | B | 306 | -25.852 | 92.987 | 12.182 | 1.00 | 51.50 | 6 |
| | ATOM | 355 | CE | LYS | B | 306 | -24.706 | 92.932 | 11.190 | 1.00 | 53.26 | 6 |
| | ATOM | 356 | NZ | LYS | B | 306 | -23.883 | 94.161 | 11.251 | 1.00 | 59.61 | 7 |
| 45 | ATOM | 357 | C | LYS | B | 306 | -24.308 | 88.484 | 13.556 | 1.00 | 35.25 | 6 |
| | ATOM | 358 | O | LYS | B | 306 | -23.681 | 87.917 | 12.653 | 1.00 | 33.95 | 8 |
| | ATOM | 359 | N | GLY | B | 307 | -23.918 | 88.478 | 14.829 | 1.00 | 35.79 | 7 |
| | ATOM | 360 | CA | GLY | B | 307 | -22.702 | 87.793 | 15.227 | 1.00 | 34.59 | 6 |
| | ATOM | 361 | C | GLY | B | 307 | -22.811 | 86.291 | 15.383 | 1.00 | 33.80 | 6 |
| 50 | ATOM | 362 | O | GLY | B | 307 | -21.944 | 85.564 | 14.895 | 1.00 | 31.59 | 8 |
| | ATOM | 363 | N | CYS | B | 308 | -23.861 | 85.843 | 16.071 | 1.00 | 31.15 | 7 |
| | ATOM | 364 | CA | CYS | B | 308 | -24.069 | 84.434 | 16.320 | 1.00 | 29.04 | 6 |
| | ATOM | 365 | CB | CYS | B | 308 | -24.761 | 84.240 | 17.663 | 1.00 | 27.59 | 6 |
| | ATOM | 366 | SG | CYS | B | 308 | -26.496 | 84.629 | 17.608 | 1.00 | 30.50 | 16 |
| 55 | ATOM | 367 | C | CYS | B | 308 | -24.911 | 83.712 | 15.266 | 1.00 | 30.59 | 6 |
| | ATOM | 368 | O | CYS | B | 308 | -25.088 | 82.499 | 15.365 | 1.00 | 33.77 | 8 |
| | ATOM | 369 | N | CYS | B | 309 | -25.432 | 84.429 | 14.266 | 1.00 | 28.46 | 7 |
| | ATOM | 370 | CA | CYS | B | 309 | -26.270 | 83.787 | 13.265 | 1.00 | 30.10 | 6 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 371 | CB | CYS | B | 309 | -26.706 | 84.761 | 12.194 | 1.00 | 33.43 | 6 |
| | ATOM | 372 | SG | CYS | B | 309 | -27.875 | 84.011 | 11.089 | 1.00 | 35.20 | 16 |
| | ATOM | 373 | C | CYS | B | 309 | -25.617 | 82.608 | 12.603 | 1.00 | 27.72 | 6 |
| | ATOM | 374 | O | CYS | B | 309 | -26.170 | 81.518 | 12.610 | 1.00 | 27.69 | 8 |
| | ATOM | 375 | N | MET | B | 310 | -24.447 | 82.829 | 12.011 | 1.00 | 26.15 | 7 |
| 10 | ATOM | 376 | CA | MET | B | 310 | -23.737 | 81.748 | 11.352 | 1.00 | 26.06 | 6 |
| | ATOM | 377 | CB | MET | B | 310 | -22.439 | 82.263 | 10.712 | 1.00 | 25.32 | 6 |
| | ATOM | 378 | CG | MET | B | 310 | -21.584 | 81.157 | 10.080 | 1.00 | 24.08 | 6 |
| | ATOM | 379 | SD | MET | B | 310 | -22.555 | 80.324 | 8.758 | 1.00 | 27.71 | 16 |
| | ATOM | 380 | CE | MET | B | 310 | -21.549 | 78.826 | 8.427 | 1.00 | 28.50 | 6 |
| 15 | ATOM | 381 | C | MET | B | 310 | -23.416 | 80.673 | 12.374 | 1.00 | 25.94 | 6 |
| | ATOM | 382 | O | MET | B | 310 | -23.659 | 79.489 | 12.151 | 1.00 | 28.09 | 8 |
| | ATOM | 383 | N | GLU | B | 311 | -22.865 | 81.117 | 13.500 | 1.00 | 25.39 | 7 |
| | ATOM | 384 | CA | GLU | B | 311 | -22.466 | 80.231 | 14.576 | 1.00 | 27.03 | 6 |
| | ATOM | 385 | CB | GLU | B | 311 | -22.036 | 81.048 | 15.797 | 1.00 | 24.39 | 6 |
| 20 | ATOM | 386 | CG | GLU | B | 311 | -21.019 | 82.141 | 15.509 | 1.00 | 26.00 | 6 |
| | ATOM | 387 | CD | GLU | B | 311 | -20.524 | 82.835 | 16.740 | 1.00 | 23.95 | 6 |
| | ATOM | 388 | OE1 | GLU | B | 311 | -21.321 | 83.108 | 17.668 | 1.00 | 19.72 | 8 |
| | ATOM | 389 | OE2 | GLU | B | 311 | -19.313 | 83.163 | 16.815 | 1.00 | 26.51 | 8 |
| | ATOM | 390 | C | GLU | B | 311 | -23.582 | 79.264 | 14.964 | 1.00 | 27.51 | 6 |
| 25 | ATOM | 391 | O | GLU | B | 311 | -23.347 | 78.068 | 15.093 | 1.00 | 29.67 | 8 |
| | ATOM | 392 | N | ILE | B | 312 | -24.794 | 79.792 | 15.145 | 1.00 | 26.82 | 7 |
| | ATOM | 393 | CA | ILE | B | 312 | -25.933 | 78.967 | 15.527 | 1.00 | 25.71 | 6 |
| | ATOM | 394 | CB | ILE | B | 312 | -27.125 | 79.814 | 16.021 | 1.00 | 23.35 | 6 |
| | ATOM | 395 | CG2 | ILE | B | 312 | -28.327 | 78.933 | 16.276 | 1.00 | 20.27 | 6 |
| 30 | ATOM | 396 | CG1 | ILE | B | 312 | -26.771 | 80.541 | 17.325 | 1.00 | 20.88 | 6 |
| | ATOM | 397 | CD1 | ILE | B | 312 | -27.952 | 81.163 | 18.028 | 1.00 | 18.15 | 6 |
| | ATOM | 398 | C | ILE | B | 312 | -26.370 | 78.072 | 14.392 | 1.00 | 27.91 | 6 |
| | ATOM | 399 | O | ILE | B | 312 | -26.769 | 76.926 | 14.605 | 1.00 | 28.96 | 8 |
| | ATOM | 400 | N | MET | B | 313 | -26.303 | 78.603 | 13.174 | 1.00 | 27.66 | 7 |
| 35 | ATOM | 401 | CA | MET | B | 313 | -26.696 | 77.832 | 11.999 | 1.00 | 30.18 | 6 |
| | ATOM | 402 | CB | MET | B | 313 | -26.696 | 78.691 | 10.734 | 1.00 | 36.89 | 6 |
| | ATOM | 403 | CG | MET | B | 313 | -27.882 | 79.634 | 10.607 | 1.00 | 37.95 | 6 |
| | ATOM | 404 | SD | MET | B | 313 | -28.238 | 80.275 | 8.907 | 1.00 | 42.38 | 16 |
| | ATOM | 405 | CE | MET | B | 313 | -26.787 | 81.316 | 8.639 | 1.00 | 40.68 | 6 |
| 40 | ATOM | 406 | C | MET | B | 313 | -25.791 | 76.632 | 11.808 | 1.00 | 27.43 | 6 |
| | ATOM | 407 | O | MET | B | 313 | -26.258 | 75.501 | 11.893 | 1.00 | 28.61 | 8 |
| | ATOM | 408 | N | SER | B | 314 | -24.508 | 76.882 | 11.549 | 1.00 | 24.88 | 7 |
| | ATOM | 409 | CA | SER | B | 314 | -23.533 | 75.824 | 11.346 | 1.00 | 27.98 | 6 |
| | ATOM | 410 | CB | SER | B | 314 | -22.150 | 76.441 | 11.165 | 1.00 | 29.64 | 6 |
| 45 | ATOM | 411 | OG | SER | B | 314 | -21.844 | 77.316 | 12.227 | 1.00 | 43.44 | 8 |
| | ATOM | 412 | C | SER | B | 314 | -23.514 | 74.774 | 12.465 | 1.00 | 22.30 | 6 |
| | ATOM | 413 | O | SER | B | 314 | -23.279 | 73.592 | 12.199 | 1.00 | 24.18 | 8 |
| | ATOM | 414 | N | LEU | B | 315 | -23.760 | 75.187 | 13.714 | 1.00 | 23.99 | 7 |
| | ATOM | 415 | CA | LEU | B | 315 | -23.792 | 74.219 | 14.811 | 1.00 | 25.07 | 6 |
| 50 | ATOM | 416 | CB | LEU | B | 315 | -24.095 | 74.869 | 16.169 | 1.00 | 19.11 | 6 |
| | ATOM | 417 | CG | LEU | B | 315 | -24.507 | 73.860 | 17.234 | 1.00 | 20.39 | 6 |
| | ATOM | 418 | CD1 | LEU | B | 315 | -23.390 | 72.878 | 17.493 | 1.00 | 18.92 | 6 |
| | ATOM | 419 | CD2 | LEU | B | 315 | -24.895 | 74.560 | 18.514 | 1.00 | 12.93 | 6 |
| | ATOM | 420 | C | LEU | B | 315 | -24.892 | 73.219 | 14.517 | 1.00 | 24.53 | 6 |
| 55 | ATOM | 421 | O | LEU | B | 315 | -24.672 | 72.014 | 14.550 | 1.00 | 26.32 | 8 |
| | ATOM | 422 | N | ARG | B | 316 | -26.079 | 73.762 | 14.254 | 1.00 | 28.18 | 7 |
| | ATOM | 423 | CA | ARG | B | 316 | -27.278 | 72.996 | 13.971 | 1.00 | 27.54 | 6 |
| | ATOM | 424 | CB | ARG | B | 316 | -28.432 | 73.941 | 13.651 | 1.00 | 27.39 | 6 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 425 | CG | ARG | B | 316 | -28.823 | 74.857 | 14.809 | 1.00 | 22.00 | 6 |
| | ATOM | 426 | CD | ARG | B | 316 | -30.074 | 75.657 | 14.451 | 1.00 | 18.78 | 6 |
| | ATOM | 427 | NE | ARG | B | 316 | -30.905 | 75.944 | 15.598 | 1.00 | 26.57 | 7 |
| | ATOM | 428 | CZ | ARG | B | 316 | -32.166 | 76.337 | 15.489 | 1.00 | 30.81 | 6 |
| | ATOM | 429 | NH1 | ARG | B | 316 | -32.686 | 76.535 | 14.280 | 1.00 | 33.71 | 7 |
| 10 | ATOM | 430 | NH2 | ARG | B | 316 | -32.900 | 76.542 | 16.581 | 1.00 | 33.13 | 7 |
| | ATOM | 431 | C | ARG | B | 316 | -27.128 | 72.028 | 12.830 | 1.00 | 28.09 | 6 |
| | ATOM | 432 | O | ARG | B | 316 | -27.852 | 71.053 | 12.760 | 1.00 | 32.41 | 8 |
| | ATOM | 433 | N | ALA | B | 317 | -26.187 | 72.309 | 11.941 | 1.00 | 28.36 | 7 |
| | ATOM | 434 | CA | ALA | B | 317 | -25.938 | 71.466 | 10.794 | 1.00 | 26.64 | 6 |
| 15 | ATOM | 435 | CB | ALA | B | 317 | -25.337 | 72.300 | 9.675 | 1.00 | 22.93 | 6 |
| | ATOM | 436 | C | ALA | B | 317 | -24.998 | 70.327 | 11.150 | 1.00 | 28.35 | 6 |
| | ATOM | 437 | O | ALA | B | 317 | -25.223 | 69.187 | 10.773 | 1.00 | 32.10 | 8 |
| | ATOM | 438 | N | ALA | B | 318 | -23.941 | 70.659 | 11.882 | 1.00 | 29.12 | 7 |
| | ATOM | 439 | CA | ALA | B | 318 | -22.957 | 69.682 | 12.299 | 1.00 | 27.50 | 6 |
| 20 | ATOM | 440 | CB | ALA | B | 318 | -21.915 | 70.355 | 13.160 | 1.00 | 28.39 | 6 |
| | ATOM | 441 | C | ALA | B | 318 | -23.645 | 68.591 | 13.084 | 1.00 | 28.10 | 6 |
| | ATOM | 442 | O | ALA | B | 318 | -23.415 | 67.415 | 12.854 | 1.00 | 28.18 | 8 |
| | ATOM | 443 | N | VAL | B | 319 | -24.502 | 69.012 | 14.016 | 1.00 | 29.16 | 7 |
| | ATOM | 444 | CA | VAL | B | 319 | -25.259 | 68.107 | 14.889 | 1.00 | 35.24 | 6 |
| 25 | ATOM | 445 | CB | VAL | B | 319 | -26.228 | 68.897 | 15.765 | 1.00 | 27.34 | 6 |
| | ATOM | 446 | CG1 | VAL | B | 319 | -25.576 | 70.149 | 16.246 | 1.00 | 29.96 | 6 |
| | ATOM | 447 | CG2 | VAL | B | 319 | -27.505 | 69.212 | 15.022 | 1.00 | 31.70 | 6 |
| | ATOM | 448 | C | VAL | B | 319 | -26.066 | 67.146 | 14.043 | 1.00 | 40.01 | 6 |
| | ATOM | 449 | O | VAL | B | 319 | -26.701 | 66.250 | 14.578 | 1.00 | 42.70 | 8 |
| 30 | ATOM | 450 | N | ARG | B | 320 | -26.025 | 67.353 | 12.723 | 1.00 | 38.64 | 7 |
| | ATOM | 451 | CA | ARG | B | 320 | -26.770 | 66.541 | 11.762 | 1.00 | 38.61 | 6 |
| | ATOM | 452 | CB | ARG | B | 320 | -27.838 | 67.409 | 11.123 | 1.00 | 37.26 | 6 |
| | ATOM | 453 | CG | ARG | B | 320 | -29.152 | 67.280 | 11.822 | 1.00 | 43.12 | 6 |
| | ATOM | 454 | CD | ARG | B | 320 | -30.145 | 68.340 | 11.387 | 1.00 | 50.79 | 6 |
| 35 | ATOM | 455 | NE | ARG | B | 320 | -31.500 | 67.911 | 11.705 | 1.00 | 54.71 | 7 |
| | ATOM | 456 | CZ | ARG | B | 320 | -32.555 | 68.723 | 11.597 | 1.00 | 57.89 | 6 |
| | ATOM | 457 | NH1 | ARG | B | 320 | -32.398 | 69.957 | 11.130 | 1.00 | 49.08 | 7 |
| | ATOM | 458 | NH2 | ARG | B | 320 | -33.773 | 68.302 | 11.844 | 1.00 | 59.59 | 7 |
| | ATOM | 459 | C | ARG | B | 320 | -25.937 | 65.910 | 10.670 | 1.00 | 42.14 | 6 |
| 40 | ATOM | 460 | O | ARG | B | 320 | -26.381 | 65.802 | 9.532 | 1.00 | 46.30 | 8 |
| | ATOM | 461 | N | TYR | B | 321 | -24.734 | 65.488 | 11.022 | 1.00 | 42.04 | 7 |
| | ATOM | 462 | CA | TYR | B | 321 | -23.858 | 64.848 | 10.063 | 1.00 | 42.70 | 6 |
| | ATOM | 463 | CB | TYR | B | 321 | -22.433 | 65.332 | 10.297 | 1.00 | 38.01 | 6 |
| | ATOM | 464 | CG | TYR | B | 321 | -21.393 | 64.396 | 9.756 | 1.00 | 37.94 | 6 |
| 45 | ATOM | 465 | CD1 | TYR | B | 321 | -21.265 | 64.176 | 8.397 | 1.00 | 33.85 | 6 |
| | ATOM | 466 | CE1 | TYR | B | 321 | -20.333 | 63.258 | 7.912 | 1.00 | 34.49 | 6 |
| | ATOM | 467 | CD2 | TYR | B | 321 | -20.583 | 63.683 | 10.613 | 1.00 | 28.03 | 6 |
| | ATOM | 468 | CE2 | TYR | B | 321 | -19.658 | 62.769 | 10.134 | 1.00 | 32.69 | 6 |
| | ATOM | 469 | CZ | TYR | B | 321 | -19.532 | 62.551 | 8.781 | 1.00 | 35.18 | 6 |
| 50 | ATOM | 470 | OH | TYR | B | 321 | -18.616 | 61.661 | 8.292 | 1.00 | 39.48 | 8 |
| | ATOM | 471 | C | TYR | B | 321 | -23.897 | 63.347 | 10.234 | 1.00 | 45.51 | 6 |
| | ATOM | 472 | O | TYR | B | 321 | -23.560 | 62.857 | 11.292 | 1.00 | 48.02 | 8 |
| | ATOM | 473 | N | ASP | B | 322 | -24.317 | 62.642 | 9.188 | 1.00 | 44.56 | 7 |
| | ATOM | 474 | CA | ASP | B | 322 | -24.391 | 61.170 | 9.182 | 1.00 | 45.86 | 6 |
| 55 | ATOM | 475 | CB | ASP | B | 322 | -25.570 | 60.749 | 8.294 | 1.00 | 46.64 | 6 |
| | ATOM | 476 | CG | ASP | B | 322 | -25.449 | 59.359 | 7.775 | 1.00 | 40.00 | 6 |
| | ATOM | 477 | OD1 | ASP | B | 322 | -24.388 | 58.737 | 7.986 | 1.00 | 40.00 | 8 |
| | ATOM | 478 | OD2 | ASP | B | 322 | -26.414 | 58.862 | 7.117 | 1.00 | 40.00 | 8 |

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|----|------|-----|-----|-----------|---------|--------|--------|------|-------|---|
| 5 | ATOM | 479 | C | ASP B 322 | -23.044 | 60.659 | 8.682 | 1.00 | 45.82 | 6 |
| | ATOM | 480 | O | ASP B 322 | -22.738 | 60.783 | 7.495 | 1.00 | 45.38 | 8 |
| | ATOM | 481 | N | PRO B 323 | -22.242 | 60.005 | 9.549 | 1.00 | 46.53 | 7 |
| | ATOM | 482 | CD | PRO B 323 | -22.594 | 59.676 | 10.934 | 1.00 | 47.16 | 6 |
| | ATOM | 483 | CA | PRO B 323 | -20.910 | 59.487 | 9.162 | 1.00 | 46.63 | 6 |
| 10 | ATOM | 484 | CB | PRO B 323 | -20.367 | 58.847 | 10.433 | 1.00 | 43.95 | 6 |
| | ATOM | 485 | CG | PRO B 323 | -21.398 | 58.958 | 11.454 | 1.00 | 43.93 | 6 |
| | ATOM | 486 | C | PRO B 323 | -20.933 | 58.489 | 8.017 | 1.00 | 48.34 | 6 |
| | ATOM | 487 | O | PRO B 323 | -20.040 | 58.457 | 7.171 | 1.00 | 50.84 | 8 |
| | ATOM | 488 | N | GLU B 324 | -21.951 | 57.631 | 8.022 | 1.00 | 52.39 | 7 |
| 15 | ATOM | 489 | CA | GLU B 324 | -22.126 | 56.615 | 7.008 | 1.00 | 55.85 | 6 |
| | ATOM | 490 | CB | GLU B 324 | -23.491 | 55.960 | 7.216 | 1.00 | 55.54 | 6 |
| | ATOM | 491 | CG | GLU B 324 | -23.678 | 55.332 | 8.581 | 1.00 | 40.00 | 6 |
| | ATOM | 492 | CD | GLU B 324 | -22.642 | 54.294 | 8.888 | 1.00 | 40.00 | 6 |
| | ATOM | 493 | OE1 | GLU B 324 | -21.796 | 53.979 | 8.000 | 1.00 | 40.00 | 8 |
| 20 | ATOM | 494 | OE2 | GLU B 324 | -22.645 | 53.751 | 10.029 | 1.00 | 40.00 | 8 |
| | ATOM | 495 | C | GLU B 324 | -22.087 | 57.292 | 5.655 | 1.00 | 54.94 | 6 |
| | ATOM | 496 | O | GLU B 324 | -21.144 | 57.149 | 4.896 | 1.00 | 59.81 | 8 |
| | ATOM | 497 | N | SER B 325 | -23.165 | 58.022 | 5.389 | 1.00 | 52.95 | 7 |
| | ATOM | 498 | CA | SER B 325 | -23.358 | 58.762 | 4.163 | 1.00 | 50.10 | 6 |
| 25 | ATOM | 499 | CB | SER B 325 | -24.768 | 59.357 | 4.163 | 1.00 | 48.23 | 6 |
| | ATOM | 500 | OG | SER B 325 | -25.051 | 59.976 | 5.403 | 1.00 | 48.71 | 8 |
| | ATOM | 501 | C | SER B 325 | -22.324 | 59.861 | 3.964 | 1.00 | 50.61 | 6 |
| | ATOM | 502 | O | SER B 325 | -21.956 | 60.176 | 2.848 | 1.00 | 52.19 | 8 |
| | ATOM | 503 | N | GLU B 326 | -21.851 | 60.422 | 5.070 | 1.00 | 45.64 | 7 |
| 30 | ATOM | 504 | CA | GLU B 326 | -20.854 | 61.476 | 5.050 | 1.00 | 43.35 | 6 |
| | ATOM | 505 | CB | GLU B 326 | -19.602 | 61.022 | 4.277 | 1.00 | 42.74 | 6 |
| | ATOM | 506 | CG | GLU B 326 | -18.880 | 59.814 | 4.876 | 1.00 | 50.32 | 6 |
| | ATOM | 507 | CD | GLU B 326 | -17.576 | 59.524 | 4.207 | 1.00 | 56.34 | 6 |
| | ATOM | 508 | OE1 | GLU B 326 | -16.898 | 58.545 | 4.608 | 1.00 | 59.31 | 8 |
| 35 | ATOM | 509 | OE2 | GLU B 326 | -17.177 | 60.255 | 3.266 | 1.00 | 55.74 | 8 |
| | ATOM | 510 | C | GLU B 326 | -21.401 | 62.731 | 4.418 | 1.00 | 40.23 | 6 |
| | ATOM | 511 | O | GLU B 326 | -20.793 | 63.285 | 3.514 | 1.00 | 40.44 | 8 |
| | ATOM | 512 | N | THR B 327 | -22.528 | 63.208 | 4.934 | 1.00 | 35.90 | 7 |
| | ATOM | 513 | CA | THR B 327 | -23.163 | 64.418 | 4.401 | 1.00 | 37.29 | 6 |
| 40 | ATOM | 514 | CB | THR B 327 | -24.146 | 64.052 | 3.285 | 1.00 | 37.63 | 6 |
| | ATOM | 515 | OG1 | THR B 327 | -25.172 | 63.199 | 3.803 | 1.00 | 38.12 | 8 |
| | ATOM | 516 | CG2 | THR B 327 | -23.445 | 63.342 | 2.130 | 1.00 | 39.90 | 6 |
| | ATOM | 517 | C | THR B 327 | -23.961 | 65.125 | 5.473 | 1.00 | 39.49 | 6 |
| | ATOM | 518 | O | THR B 327 | -24.645 | 64.473 | 6.264 | 1.00 | 40.50 | 8 |
| 45 | ATOM | 519 | N | LEU B 328 | -23.909 | 66.454 | 5.473 | 1.00 | 36.64 | 7 |
| | ATOM | 520 | CA | LEU B 328 | -24.675 | 67.239 | 6.447 | 1.00 | 37.73 | 6 |
| | ATOM | 521 | CB | LEU B 328 | -24.061 | 68.637 | 6.620 | 1.00 | 37.78 | 6 |
| | ATOM | 522 | CG | LEU B 328 | -22.586 | 68.750 | 6.931 | 1.00 | 36.26 | 6 |
| | ATOM | 523 | CD1 | LEU B 328 | -22.260 | 70.145 | 7.411 | 1.00 | 36.56 | 6 |
| 50 | ATOM | 524 | CD2 | LEU B 328 | -22.231 | 67.751 | 8.000 | 1.00 | 39.85 | 6 |
| | ATOM | 525 | C | LEU B 328 | -26.090 | 67.344 | 5.897 | 1.00 | 37.27 | 6 |
| | ATOM | 526 | O | LEU B 328 | -26.358 | 66.855 | 4.805 | 1.00 | 34.96 | 8 |
| | ATOM | 527 | N | THR B 329 | -26.989 | 67.975 | 6.647 | 1.00 | 39.73 | 7 |
| | ATOM | 528 | CA | THR B 329 | -28.369 | 68.132 | 6.215 | 1.00 | 40.81 | 6 |
| 55 | ATOM | 529 | CB | THR B 329 | -29.279 | 67.135 | 6.918 | 1.00 | 42.67 | 6 |
| | ATOM | 530 | OG1 | THR B 329 | -28.799 | 65.809 | 6.686 | 1.00 | 42.52 | 8 |
| | ATOM | 531 | CG2 | THR B 329 | -30.702 | 67.255 | 6.375 | 1.00 | 43.52 | 6 |
| | ATOM | 532 | C | THR B 329 | -28.853 | 69.529 | 6.498 | 1.00 | 44.31 | 6 |

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|----|------|-----|-----|-----------|---------|--------|--------|------|-------|----|
| 5 | ATOM | 533 | O | THR B 329 | -29.432 | 69.801 | 7.535 | 1.00 | 43.72 | 8 |
| | ATOM | 534 | N | LEU B 330 | -28.589 | 70.413 | 5.546 | 1.00 | 44.62 | 7 |
| | ATOM | 535 | CA | LEU B 330 | -28.983 | 71.812 | 5.658 | 1.00 | 45.09 | 6 |
| | ATOM | 536 | CB | LEU B 330 | -28.354 | 72.608 | 4.510 | 1.00 | 44.66 | 6 |
| | ATOM | 537 | CG | LEU B 330 | -26.847 | 72.735 | 4.539 | 1.00 | 51.06 | 6 |
| 10 | ATOM | 538 | CD1 | LEU B 330 | -26.226 | 71.367 | 4.640 | 1.00 | 48.58 | 6 |
| | ATOM | 539 | CD2 | LEU B 330 | -26.364 | 73.450 | 3.299 | 1.00 | 45.18 | 6 |
| | ATOM | 540 | C | LEU B 330 | -30.508 | 71.965 | 5.652 | 1.00 | 48.06 | 6 |
| | ATOM | 541 | O | LEU B 330 | -31.211 | 71.244 | 4.959 | 1.00 | 49.33 | 8 |
| | ATOM | 542 | N | ASN B 331 | -30.988 | 72.911 | 6.458 | 1.00 | 52.20 | 7 |
| 15 | ATOM | 543 | CA | ASN B 331 | -32.407 | 73.214 | 6.588 | 1.00 | 54.41 | 6 |
| | ATOM | 544 | CB | ASN B 331 | -32.870 | 74.013 | 5.370 | 1.00 | 54.94 | 6 |
| | ATOM | 545 | CG | ASN B 331 | -33.687 | 75.220 | 5.749 | 1.00 | 60.35 | 6 |
| | ATOM | 546 | OD1 | ASN B 331 | -33.182 | 76.130 | 6.430 | 1.00 | 61.84 | 8 |
| | ATOM | 547 | ND2 | ASN B 331 | -34.935 | 75.242 | 5.324 | 1.00 | 65.92 | 7 |
| 20 | ATOM | 548 | C | ASN B 331 | -33.251 | 71.959 | 6.731 | 1.00 | 58.00 | 6 |
| | ATOM | 549 | O | ASN B 331 | -34.464 | 72.000 | 6.579 | 1.00 | 60.17 | 8 |
| | ATOM | 550 | N | GLY B 332 | -32.596 | 70.846 | 7.054 | 1.00 | 58.45 | 7 |
| | ATOM | 551 | CA | GLY B 332 | -33.295 | 69.587 | 7.235 | 1.00 | 58.55 | 6 |
| | ATOM | 552 | C | GLY B 332 | -33.909 | 69.004 | 5.984 | 1.00 | 59.79 | 6 |
| 25 | ATOM | 553 | O | GLY B 332 | -34.609 | 68.000 | 6.065 | 1.00 | 61.32 | 8 |
| | ATOM | 554 | N | GLU B 333 | -33.639 | 69.628 | 4.838 | 1.00 | 60.28 | 7 |
| | ATOM | 555 | CA | GLU B 333 | -34.196 | 69.182 | 3.571 | 1.00 | 59.13 | 6 |
| | ATOM | 556 | CB | GLU B 333 | -34.966 | 70.323 | 2.885 | 1.00 | 62.40 | 6 |
| | ATOM | 557 | CG | GLU B 333 | -36.099 | 70.963 | 3.690 | 1.00 | 75.69 | 6 |
| 30 | ATOM | 558 | CD | GLU B 333 | -36.720 | 72.135 | 2.998 | 1.00 | 80.41 | 6 |
| | ATOM | 559 | OE1 | GLU B 333 | -35.984 | 73.081 | 2.618 | 1.00 | 79.98 | 8 |
| | ATOM | 560 | OE2 | GLU B 333 | -37.966 | 72.158 | 2.830 | 1.00 | 83.81 | 8 |
| | ATOM | 561 | C | GLU B 333 | -33.110 | 68.722 | 2.624 | 1.00 | 57.18 | 6 |
| | ATOM | 562 | O | GLU B 333 | -33.236 | 67.689 | 1.974 | 1.00 | 57.50 | 8 |
| 35 | ATOM | 563 | N | MET B 334 | -32.054 | 69.528 | 2.539 | 1.00 | 55.20 | 7 |
| | ATOM | 564 | CA | MET B 334 | -30.926 | 69.259 | 1.653 | 1.00 | 50.85 | 6 |
| | ATOM | 565 | CB | MET B 334 | -30.514 | 70.563 | 0.984 | 1.00 | 48.70 | 6 |
| | ATOM | 566 | CG | MET B 334 | -29.244 | 70.460 | 0.194 | 1.00 | 45.39 | 6 |
| | ATOM | 567 | SD | MET B 334 | -28.743 | 72.008 | -0.624 | 1.00 | 44.56 | 16 |
| 40 | ATOM | 568 | CE | MET B 334 | -30.307 | 72.445 | -1.503 | 1.00 | 45.25 | 6 |
| | ATOM | 569 | C | MET B 334 | -29.711 | 68.634 | 2.319 | 1.00 | 51.59 | 6 |
| | ATOM | 570 | O | MET B 334 | -29.185 | 69.161 | 3.291 | 1.00 | 52.52 | 8 |
| | ATOM | 571 | N | ALA B 335 | -29.270 | 67.515 | 1.758 | 1.00 | 51.00 | 7 |
| | ATOM | 572 | CA | ALA B 335 | -28.106 | 66.802 | 2.267 | 1.00 | 48.98 | 6 |
| 45 | ATOM | 573 | CB | ALA B 335 | -28.377 | 65.304 | 2.274 | 1.00 | 47.86 | 6 |
| | ATOM | 574 | C | ALA B 335 | -26.931 | 67.108 | 1.371 | 1.00 | 51.01 | 6 |
| | ATOM | 575 | O | ALA B 335 | -26.936 | 66.760 | 0.190 | 1.00 | 51.61 | 8 |
| | ATOM | 576 | N | VAL B 336 | -25.921 | 67.770 | 1.930 | 1.00 | 46.62 | 7 |
| | ATOM | 577 | CA | VAL B 336 | -24.730 | 68.142 | 1.152 | 1.00 | 42.35 | 6 |
| 50 | ATOM | 578 | CB | VAL B 336 | -24.466 | 69.635 | 1.258 | 1.00 | 42.41 | 6 |
| | ATOM | 579 | CG1 | VAL B 336 | -25.695 | 70.418 | 0.860 | 1.00 | 42.00 | 6 |
| | ATOM | 580 | CG2 | VAL B 336 | -24.018 | 70.004 | 2.642 | 1.00 | 40.32 | 6 |
| | ATOM | 581 | C | VAL B 336 | -23.493 | 67.390 | 1.611 | 1.00 | 45.33 | 6 |
| | ATOM | 582 | O | VAL B 336 | -23.464 | 66.775 | 2.681 | 1.00 | 47.42 | 8 |
| 55 | ATOM | 583 | N | THR B 337 | -22.461 | 67.478 | 0.781 | 1.00 | 41.60 | 7 |
| | ATOM | 584 | CA | THR B 337 | -21.172 | 66.818 | 1.041 | 1.00 | 39.69 | 6 |
| | ATOM | 585 | CB | THR B 337 | -20.720 | 66.011 | -0.173 | 1.00 | 41.35 | 6 |
| | ATOM | 586 | OG1 | THR B 337 | -20.273 | 66.887 | -1.213 | 1.00 | 49.35 | 8 |

| | | | | | | | | | | | | |
|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 587 | CG2 | THR | B | 337 | -21.869 | 65.175 | -0.702 | 1.00 | 40.38 | 6 |
| | ATOM | 588 | C | THR | B | 337 | -20.087 | 67.846 | 1.318 | 1.00 | 37.88 | 6 |
| | ATOM | 589 | O | THR | B | 337 | -20.141 | 68.975 | 0.832 | 1.00 | 34.06 | 8 |
| | ATOM | 590 | N | ARG | B | 338 | -19.097 | 67.417 | 2.095 | 1.00 | 37.61 | 7 |
| | ATOM | 591 | CA | ARG | B | 338 | -17.942 | 68.241 | 2.442 | 1.00 | 38.68 | 6 |
| 10 | ATOM | 592 | CB | ARG | B | 338 | -16.770 | 67.333 | 2.823 | 1.00 | 35.95 | 6 |
| | ATOM | 593 | CG | ARG | B | 338 | -15.455 | 68.042 | 3.064 | 1.00 | 38.83 | 6 |
| | ATOM | 594 | CD | ARG | B | 338 | -14.348 | 67.029 | 3.319 | 1.00 | 35.88 | 6 |
| | ATOM | 595 | NE | ARG | B | 338 | -14.520 | 66.239 | 4.530 | 1.00 | 37.42 | 7 |
| | ATOM | 596 | CZ | ARG | B | 338 | -14.274 | 66.669 | 5.766 | 1.00 | 30.20 | 6 |
| 15 | ATOM | 597 | NH1 | ARG | B | 338 | -13.794 | 67.892 | 5.973 | 1.00 | 27.98 | 7 |
| | ATOM | 598 | NH2 | ARG | B | 338 | -14.481 | 65.847 | 6.788 | 1.00 | 27.40 | 7 |
| | ATOM | 599 | C | ARG | B | 338 | -17.581 | 69.075 | 1.229 | 1.00 | 38.09 | 6 |
| | ATOM | 600 | O | ARG | B | 338 | -17.537 | 70.299 | 1.284 | 1.00 | 34.12 | 8 |
| | ATOM | 601 | N | GLY | B | 339 | -17.345 | 68.383 | 0.117 | 1.00 | 41.25 | 7 |
| 20 | ATOM | 602 | CA | GLY | B | 339 | -16.981 | 69.054 | -1.119 | 1.00 | 41.35 | 6 |
| | ATOM | 603 | C | GLY | B | 339 | -18.004 | 70.109 | -1.460 | 1.00 | 41.23 | 6 |
| | ATOM | 604 | O | GLY | B | 339 | -17.736 | 71.291 | -1.330 | 1.00 | 38.30 | 8 |
| | ATOM | 605 | N | GLN | B | 340 | -19.174 | 69.665 | -1.909 | 1.00 | 38.58 | 7 |
| | ATOM | 606 | CA | GLN | B | 340 | -20.258 | 70.564 | -2.276 | 1.00 | 40.79 | 6 |
| 25 | ATOM | 607 | CB | GLN | B | 340 | -21.596 | 69.843 | -2.079 | 1.00 | 40.82 | 6 |
| | ATOM | 608 | CG | GLN | B | 340 | -21.830 | 68.657 | -3.029 | 1.00 | 41.10 | 6 |
| | ATOM | 609 | CD | GLN | B | 340 | -23.154 | 67.937 | -2.783 | 1.00 | 48.84 | 6 |
| | ATOM | 610 | OE1 | GLN | B | 340 | -23.353 | 67.313 | -1.715 | 1.00 | 50.53 | 8 |
| | ATOM | 611 | NE2 | GLN | B | 340 | -24.050 | 68.015 | -3.753 | 1.00 | 54.25 | 7 |
| 30 | ATOM | 612 | C | GLN | B | 340 | -20.239 | 71.872 | -1.475 | 1.00 | 41.50 | 6 |
| | ATOM | 613 | O | GLN | B | 340 | -20.114 | 72.958 | -2.032 | 1.00 | 42.72 | 8 |
| | ATOM | 614 | N | LEU | B | 341 | -20.352 | 71.736 | -0.156 | 1.00 | 42.00 | 7 |
| | ATOM | 615 | CA | LEU | B | 341 | -20.375 | 72.879 | 0.746 | 1.00 | 38.10 | 6 |
| | ATOM | 616 | CB | LEU | B | 341 | -20.401 | 72.419 | 2.201 | 1.00 | 36.66 | 6 |
| 35 | ATOM | 617 | CG | LEU | B | 341 | -20.678 | 73.514 | 3.194 | 1.00 | 39.94 | 6 |
| | ATOM | 618 | CD1 | LEU | B | 341 | -22.088 | 74.038 | 2.936 | 1.00 | 34.98 | 6 |
| | ATOM | 619 | CD2 | LEU | B | 341 | -20.570 | 72.990 | 4.609 | 1.00 | 40.95 | 6 |
| | ATOM | 620 | C | LEU | B | 341 | -19.170 | 73.763 | 0.543 | 1.00 | 36.37 | 6 |
| | ATOM | 621 | O | LEU | B | 341 | -19.293 | 74.974 | 0.497 | 1.00 | 37.89 | 8 |
| 40 | ATOM | 622 | N | LYS | B | 342 | -18.003 | 73.136 | 0.433 | 1.00 | 33.29 | 7 |
| | ATOM | 623 | CA | LYS | B | 342 | -16.737 | 73.843 | 0.239 | 1.00 | 35.17 | 6 |
| | ATOM | 624 | CB | LYS | B | 342 | -15.603 | 72.821 | 0.176 | 1.00 | 34.97 | 6 |
| | ATOM | 625 | CG | LYS | B | 342 | -14.210 | 73.401 | 0.306 | 1.00 | 40.00 | 6 |
| | ATOM | 626 | CD | LYS | B | 342 | -13.155 | 72.288 | 0.316 | 1.00 | 34.48 | 6 |
| 45 | ATOM | 627 | CE | LYS | B | 342 | -11.775 | 72.809 | 0.755 | 1.00 | 37.54 | 6 |
| | ATOM | 628 | NZ | LYS | B | 342 | -10.790 | 71.680 | 0.981 | 1.00 | 42.32 | 7 |
| | ATOM | 629 | C | LYS | B | 342 | -16.744 | 74.685 | -1.038 | 1.00 | 38.29 | 6 |
| | ATOM | 630 | O | LYS | B | 342 | -16.725 | 75.911 | -0.993 | 1.00 | 36.23 | 8 |
| | ATOM | 631 | N | ASN | B | 343 | -16.760 | 73.990 | -2.172 | 1.00 | 39.25 | 7 |
| 50 | ATOM | 632 | CA | ASN | B | 343 | -16.762 | 74.609 | -3.481 | 1.00 | 40.19 | 6 |
| | ATOM | 633 | CB | ASN | B | 343 | -16.977 | 73.539 | -4.551 | 1.00 | 37.96 | 6 |
| | ATOM | 634 | CG | ASN | B | 343 | -16.178 | 72.272 | -4.277 | 1.00 | 39.22 | 6 |
| | ATOM | 635 | OD1 | ASN | B | 343 | -14.938 | 72.313 | -4.106 | 1.00 | 42.37 | 8 |
| | ATOM | 636 | ND2 | ASN | B | 343 | -16.877 | 71.144 | -4.259 | 1.00 | 42.19 | 7 |
| 55 | ATOM | 637 | C | ASN | B | 343 | -17.894 | 75.624 | -3.547 | 1.00 | 40.12 | 6 |
| | ATOM | 638 | O | ASN | B | 343 | -17.835 | 76.600 | -4.284 | 1.00 | 36.01 | 8 |
| | ATOM | 639 | N | GLY | B | 344 | -18.934 | 75.361 | -2.756 | 1.00 | 40.95 | 7 |
| | ATOM | 640 | CA | GLY | B | 344 | -20.101 | 76.222 | -2.709 | 1.00 | 39.25 | 6 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 641 | C | GLY | B | 344 | -19.867 | 77.636 | -2.258 | 1.00 | 38.26 | 6 |
| | ATOM | 642 | O | GLY | B | 344 | -20.715 | 78.501 | -2.484 | 1.00 | 35.69 | 8 |
| | ATOM | 643 | N | GLY | B | 345 | -18.724 | 77.871 | -1.619 | 1.00 | 35.89 | 7 |
| | ATOM | 644 | CA | GLY | B | 345 | -18.426 | 79.209 | -1.159 | 1.00 | 34.00 | 6 |
| | ATOM | 645 | C | GLY | B | 345 | -17.848 | 79.298 | 0.230 | 1.00 | 38.64 | 6 |
| 10 | ATOM | 646 | O | GLY | B | 345 | -17.216 | 80.303 | 0.573 | 1.00 | 38.14 | 8 |
| | ATOM | 647 | N | LEU | B | 346 | -18.071 | 78.266 | 1.041 | 1.00 | 39.52 | 7 |
| | ATOM | 648 | CA | LEU | B | 346 | -17.563 | 78.279 | 2.403 | 1.00 | 36.05 | 6 |
| | ATOM | 649 | CB | LEU | B | 346 | -18.311 | 77.256 | 3.269 | 1.00 | 35.72 | 6 |
| | ATOM | 650 | CG | LEU | B | 346 | -19.800 | 77.473 | 3.378 | 1.00 | 34.89 | 6 |
| 15 | ATOM | 651 | CD1 | LEU | B | 346 | -20.322 | 76.678 | 4.554 | 1.00 | 44.09 | 6 |
| | ATOM | 652 | CD2 | LEU | B | 346 | -20.086 | 78.937 | 3.612 | 1.00 | 34.84 | 6 |
| | ATOM | 653 | C | LEU | B | 346 | -16.079 | 78.018 | 2.445 | 1.00 | 33.52 | 6 |
| | ATOM | 654 | O | LEU | B | 346 | -15.392 | 78.387 | 3.394 | 1.00 | 35.58 | 8 |
| | ATOM | 655 | N | GLY | B | 347 | -15.586 | 77.388 | 1.385 | 1.00 | 30.47 | 7 |
| 20 | ATOM | 656 | CA | GLY | B | 347 | -14.174 | 77.078 | 1.305 | 1.00 | 33.01 | 6 |
| | ATOM | 657 | C | GLY | B | 347 | -13.768 | 76.214 | 2.477 | 1.00 | 30.72 | 6 |
| | ATOM | 658 | O | GLY | B | 347 | -14.433 | 75.243 | 2.808 | 1.00 | 30.89 | 8 |
| | ATOM | 659 | N | VAL | B | 348 | -12.647 | 76.585 | 3.087 | 1.00 | 31.30 | 7 |
| | ATOM | 660 | CA | VAL | B | 348 | -12.097 | 75.867 | 4.227 | 1.00 | 31.27 | 6 |
| 25 | ATOM | 661 | CB | VAL | B | 348 | -10.889 | 76.609 | 4.817 | 1.00 | 31.66 | 6 |
| | ATOM | 662 | CG1 | VAL | B | 348 | -11.292 | 77.974 | 5.360 | 1.00 | 20.19 | 6 |
| | ATOM | 663 | CG2 | VAL | B | 348 | -10.250 | 75.786 | 5.905 | 1.00 | 24.77 | 6 |
| | ATOM | 664 | C | VAL | B | 348 | -13.136 | 75.651 | 5.360 | 1.00 | 33.84 | 6 |
| | ATOM | 665 | O | VAL | B | 348 | -13.002 | 74.707 | 6.153 | 1.00 | 29.99 | 8 |
| 30 | ATOM | 666 | N | VAL | B | 349 | -14.157 | 76.518 | 5.449 | 1.00 | 33.31 | 7 |
| | ATOM | 667 | CA | VAL | B | 349 | -15.147 | 76.339 | 6.483 | 1.00 | 32.23 | 6 |
| | ATOM | 668 | CB | VAL | B | 349 | -16.226 | 77.393 | 6.476 | 1.00 | 32.59 | 6 |
| | ATOM | 669 | CG1 | VAL | B | 349 | -17.342 | 76.979 | 7.399 | 1.00 | 33.68 | 6 |
| | ATOM | 670 | CG2 | VAL | B | 349 | -15.667 | 78.703 | 6.959 | 1.00 | 32.30 | 6 |
| 35 | ATOM | 671 | C | VAL | B | 349 | -15.792 | 74.987 | 6.380 | 1.00 | 34.91 | 6 |
| | ATOM | 672 | O | VAL | B | 349 | -16.055 | 74.359 | 7.394 | 1.00 | 33.73 | 8 |
| | ATOM | 673 | N | SER | B | 350 | -16.054 | 74.507 | 5.176 | 1.00 | 32.81 | 7 |
| | ATOM | 674 | CA | SER | B | 350 | -16.695 | 73.215 | 5.100 | 1.00 | 30.10 | 6 |
| | ATOM | 675 | CB | SER | B | 350 | -16.772 | 72.697 | 3.684 | 1.00 | 24.95 | 6 |
| 40 | ATOM | 676 | OG | SER | B | 350 | -17.538 | 71.502 | 3.644 | 1.00 | 23.16 | 8 |
| | ATOM | 677 | C | SER | B | 350 | -15.910 | 72.254 | 5.942 | 1.00 | 31.59 | 6 |
| | ATOM | 678 | O | SER | B | 350 | -16.417 | 71.807 | 6.950 | 1.00 | 37.62 | 8 |
| | ATOM | 679 | N | ASP | B | 351 | -14.675 | 71.942 | 5.565 | 1.00 | 28.60 | 7 |
| | ATOM | 680 | CA | ASP | B | 351 | -13.905 | 71.010 | 6.378 | 1.00 | 29.82 | 6 |
| 45 | ATOM | 681 | CB | ASP | B | 351 | -12.419 | 71.139 | 6.050 | 1.00 | 27.49 | 6 |
| | ATOM | 682 | CG | ASP | B | 351 | -12.151 | 71.094 | 4.585 | 1.00 | 30.22 | 6 |
| | ATOM | 683 | OD1 | ASP | B | 351 | -12.013 | 72.174 | 3.954 | 1.00 | 32.61 | 8 |
| | ATOM | 684 | OD2 | ASP | B | 351 | -12.064 | 69.980 | 4.017 | 1.00 | 30.02 | 8 |
| | ATOM | 685 | C | ASP | B | 351 | -14.176 | 71.343 | 7.861 | 1.00 | 30.63 | 6 |
| 50 | ATOM | 686 | O | ASP | B | 351 | -14.458 | 70.474 | 8.681 | 1.00 | 29.54 | 8 |
| | ATOM | 687 | N | ALA | B | 352 | -14.111 | 72.629 | 8.177 | 1.00 | 25.33 | 7 |
| | ATOM | 688 | CA | ALA | B | 352 | -14.346 | 73.092 | 9.533 | 1.00 | 28.59 | 6 |
| | ATOM | 689 | CB | ALA | B | 352 | -14.252 | 74.606 | 9.572 | 1.00 | 20.95 | 6 |
| | ATOM | 690 | C | ALA | B | 352 | -15.690 | 72.630 | 10.086 | 1.00 | 29.69 | 6 |
| 55 | ATOM | 691 | O | ALA | B | 352 | -15.757 | 72.068 | 11.164 | 1.00 | 30.36 | 8 |
| | ATOM | 692 | N | ILE | B | 353 | -16.754 | 72.884 | 9.330 | 1.00 | 27.63 | 7 |
| | ATOM | 693 | CA | ILE | B | 353 | -18.096 | 72.506 | 9.729 | 1.00 | 27.55 | 6 |
| | ATOM | 694 | CB | ILE | B | 353 | -19.144 | 73.129 | 8.800 | 1.00 | 28.04 | 6 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 695 | CG2 | ILE | B | 353 | -20.529 | 72.673 | 9.195 | 1.00 | 23.68 | 6 |
| | ATOM | 696 | CG1 | ILE | B | 353 | -19.108 | 74.657 | 8.869 | 1.00 | 27.33 | 6 |
| | ATOM | 697 | CD1 | ILE | B | 353 | -20.141 | 75.313 | 7.964 | 1.00 | 26.23 | 6 |
| | ATOM | 698 | C | ILE | B | 353 | -18.309 | 71.002 | 9.775 | 1.00 | 30.88 | 6 |
| | ATOM | 699 | O | ILE | B | 353 | -19.021 | 70.499 | 10.639 | 1.00 | 31.22 | 8 |
| 10 | ATOM | 700 | N | PHE | B | 354 | -17.728 | 70.279 | 8.822 | 1.00 | 29.86 | 7 |
| | ATOM | 701 | CA | PHE | B | 354 | -17.881 | 68.831 | 8.797 | 1.00 | 31.08 | 6 |
| | ATOM | 702 | CB | PHE | B | 354 | -17.461 | 68.249 | 7.439 | 1.00 | 28.80 | 6 |
| | ATOM | 703 | CG | PHE | B | 354 | -18.568 | 68.233 | 6.405 | 1.00 | 28.80 | 6 |
| | ATOM | 704 | CD1 | PHE | B | 354 | -19.031 | 69.403 | 5.833 | 1.00 | 30.96 | 6 |
| 15 | ATOM | 705 | CD2 | PHE | B | 354 | -19.150 | 67.027 | 6.034 | 1.00 | 29.45 | 6 |
| | ATOM | 706 | CE1 | PHE | B | 354 | -20.066 | 69.362 | 4.902 | 1.00 | 27.12 | 6 |
| | ATOM | 707 | CE2 | PHE | B | 354 | -20.186 | 66.978 | 5.104 | 1.00 | 25.19 | 6 |
| | ATOM | 708 | CZ | PHE | B | 354 | -20.644 | 68.146 | 4.535 | 1.00 | 28.09 | 6 |
| | ATOM | 709 | C | PHE | B | 354 | -17.041 | 68.223 | 9.913 | 1.00 | 29.17 | 6 |
| 20 | ATOM | 710 | O | PHE | B | 354 | -17.544 | 67.429 | 10.700 | 1.00 | 32.62 | 8 |
| | ATOM | 711 | N | ASP | B | 355 | -15.761 | 68.593 | 9.972 | 1.00 | 23.86 | 7 |
| | ATOM | 712 | CA | ASP | B | 355 | -14.864 | 68.090 | 11.005 | 1.00 | 25.34 | 6 |
| | ATOM | 713 | CB | ASP | B | 355 | -13.582 | 68.929 | 11.045 | 1.00 | 21.41 | 6 |
| | ATOM | 714 | CG | ASP | B | 355 | -12.548 | 68.456 | 10.086 | 1.00 | 32.08 | 6 |
| 25 | ATOM | 715 | OD1 | ASP | B | 355 | -12.899 | 68.069 | 8.944 | 1.00 | 33.58 | 8 |
| | ATOM | 716 | OD2 | ASP | B | 355 | -11.345 | 68.477 | 10.450 | 1.00 | 33.20 | 8 |
| | ATOM | 717 | C | ASP | B | 355 | -15.570 | 68.153 | 12.357 | 1.00 | 27.86 | 6 |
| | ATOM | 718 | O | ASP | B | 355 | -15.430 | 67.257 | 13.182 | 1.00 | 32.42 | 8 |
| | ATOM | 719 | N | LEU | B | 356 | -16.339 | 69.223 | 12.561 | 1.00 | 26.84 | 7 |
| 30 | ATOM | 720 | CA | LEU | B | 356 | -17.085 | 69.400 | 13.803 | 1.00 | 28.66 | 6 |
| | ATOM | 721 | CB | LEU | B | 356 | -17.832 | 70.742 | 13.800 | 1.00 | 25.37 | 6 |
| | ATOM | 722 | CG | LEU | B | 356 | -18.655 | 71.091 | 15.023 | 1.00 | 27.61 | 6 |
| | ATOM | 723 | CD1 | LEU | B | 356 | -17.729 | 71.248 | 16.191 | 1.00 | 25.43 | 6 |
| | ATOM | 724 | CD2 | LEU | B | 356 | -19.430 | 72.363 | 14.808 | 1.00 | 27.49 | 6 |
| 35 | ATOM | 725 | C | LEU | B | 356 | -18.084 | 68.260 | 13.883 | 1.00 | 30.44 | 6 |
| | ATOM | 726 | O | LEU | B | 356 | -18.054 | 67.445 | 14.804 | 1.00 | 31.55 | 8 |
| | ATOM | 727 | N | GLY | B | 357 | -18.972 | 68.214 | 12.891 | 1.00 | 32.69 | 7 |
| | ATOM | 728 | CA | GLY | B | 357 | -20.001 | 67.186 | 12.846 | 1.00 | 29.87 | 6 |
| | ATOM | 729 | C | GLY | B | 357 | -19.486 | 65.832 | 13.279 | 1.00 | 33.12 | 6 |
| 40 | ATOM | 730 | O | GLY | B | 357 | -20.032 | 65.246 | 14.207 | 1.00 | 29.41 | 8 |
| | ATOM | 731 | N | MET | B | 358 | -18.444 | 65.351 | 12.593 | 1.00 | 33.31 | 7 |
| | ATOM | 732 | CA | MET | B | 358 | -17.834 | 64.066 | 12.902 | 1.00 | 35.87 | 6 |
| | ATOM | 733 | CB | MET | B | 358 | -16.513 | 63.903 | 12.151 | 1.00 | 34.56 | 6 |
| | ATOM | 734 | CG | MET | B | 358 | -16.649 | 63.908 | 10.657 | 1.00 | 46.43 | 6 |
| 45 | ATOM | 735 | SD | MET | B | 358 | -15.094 | 63.597 | 9.751 | 1.00 | 42.13 | 16 |
| | ATOM | 736 | CE | MET | B | 358 | -14.121 | 65.063 | 10.228 | 1.00 | 44.29 | 6 |
| | ATOM | 737 | C | MET | B | 358 | -17.552 | 63.976 | 14.392 | 1.00 | 33.26 | 6 |
| | ATOM | 738 | O | MET | B | 358 | -18.019 | 63.075 | 15.075 | 1.00 | 36.39 | 8 |
| | ATOM | 739 | N | SER | B | 359 | -16.766 | 64.933 | 14.875 | 1.00 | 33.31 | 7 |
| 50 | ATOM | 740 | CA | SER | B | 359 | -16.380 | 64.998 | 16.270 | 1.00 | 34.39 | 6 |
| | ATOM | 741 | CB | SER | B | 359 | -15.724 | 66.339 | 16.541 | 1.00 | 30.84 | 6 |
| | ATOM | 742 | OG | SER | B | 359 | -15.130 | 66.355 | 17.825 | 1.00 | 47.14 | 8 |
| | ATOM | 743 | C | SER | B | 359 | -17.579 | 64.813 | 17.169 | 1.00 | 36.43 | 6 |
| | ATOM | 744 | O | SER | B | 359 | -17.635 | 63.853 | 17.922 | 1.00 | 35.46 | 8 |
| 55 | ATOM | 745 | N | LEU | B | 360 | -18.525 | 65.744 | 17.079 | 1.00 | 36.74 | 7 |
| | ATOM | 746 | CA | LEU | B | 360 | -19.741 | 65.729 | 17.889 | 1.00 | 35.44 | 6 |
| | ATOM | 747 | CB | LEU | B | 360 | -20.706 | 66.817 | 17.405 | 1.00 | 34.16 | 6 |
| | ATOM | 748 | CG | LEU | B | 360 | -20.263 | 68.255 | 17.575 | 1.00 | 34.59 | 6 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 749 | CD1 | LEU | B | 360 | -21.394 | 69.181 | 17.212 | 1.00 | 33.53 | 6 |
| | ATOM | 750 | CD2 | LEU | B | 360 | -19.869 | 68.486 | 19.010 | 1.00 | 31.69 | 6 |
| | ATOM | 751 | C | LEU | B | 360 | -20.464 | 64.397 | 17.924 | 1.00 | 38.72 | 6 |
| | ATOM | 752 | O | LEU | B | 360 | -21.021 | 64.011 | 18.958 | 1.00 | 38.29 | 8 |
| | ATOM | 753 | N | SER | B | 361 | -20.466 | 63.708 | 16.791 | 1.00 | 40.96 | 7 |
| 10 | ATOM | 754 | CA | SER | B | 361 | -21.106 | 62.416 | 16.721 | 1.00 | 45.67 | 6 |
| | ATOM | 755 | CB | SER | B | 361 | -20.532 | 61.630 | 15.551 | 1.00 | 46.45 | 6 |
| | ATOM | 756 | OG | SER | B | 361 | -20.750 | 62.314 | 14.322 | 1.00 | 51.81 | 8 |
| | ATOM | 757 | C | SER | B | 361 | -20.895 | 61.638 | 18.018 | 1.00 | 44.49 | 6 |
| | ATOM | 758 | O | SER | B | 361 | -21.696 | 60.793 | 18.362 | 1.00 | 46.67 | 8 |
| 15 | ATOM | 759 | N | SER | B | 362 | -19.811 | 61.953 | 18.726 | 1.00 | 41.44 | 7 |
| | ATOM | 760 | CA | SER | B | 362 | -19.453 | 61.309 | 19.972 | 1.00 | 42.13 | 6 |
| | ATOM | 761 | CB | SER | B | 362 | -17.962 | 61.510 | 20.234 | 1.00 | 42.61 | 6 |
| | ATOM | 762 | OG | SER | B | 362 | -17.164 | 61.025 | 19.158 | 1.00 | 51.87 | 8 |
| | ATOM | 763 | C | SER | B | 362 | -20.228 | 61.812 | 21.174 | 1.00 | 38.41 | 6 |
| 20 | ATOM | 764 | O | SER | B | 362 | -20.602 | 61.025 | 22.035 | 1.00 | 38.01 | 8 |
| | ATOM | 765 | N | PHE | B | 363 | -20.455 | 63.123 | 21.228 | 1.00 | 34.55 | 7 |
| | ATOM | 766 | CA | PHE | B | 363 | -21.150 | 63.735 | 22.346 | 1.00 | 32.96 | 6 |
| | ATOM | 767 | CB | PHE | B | 363 | -21.006 | 65.245 | 22.285 | 1.00 | 31.99 | 6 |
| | ATOM | 768 | CG | PHE | B | 363 | -19.578 | 65.719 | 22.378 | 1.00 | 29.97 | 6 |
| 25 | ATOM | 769 | CD1 | PHE | B | 363 | -19.286 | 67.058 | 22.447 | 1.00 | 30.61 | 6 |
| | ATOM | 770 | CD2 | PHE | B | 363 | -18.536 | 64.800 | 22.391 | 1.00 | 32.02 | 6 |
| | ATOM | 771 | CE1 | PHE | B | 363 | -17.966 | 67.489 | 22.543 | 1.00 | 33.67 | 6 |
| | ATOM | 772 | CE2 | PHE | B | 363 | -17.221 | 65.222 | 22.484 | 1.00 | 30.91 | 6 |
| | ATOM | 773 | CZ | PHE | B | 363 | -16.927 | 66.557 | 22.554 | 1.00 | 29.33 | 6 |
| 30 | ATOM | 774 | C | PHE | B | 363 | -22.617 | 63.361 | 22.482 | 1.00 | 30.52 | 6 |
| | ATOM | 775 | O | PHE | B | 363 | -23.142 | 63.331 | 23.596 | 1.00 | 32.19 | 8 |
| | ATOM | 776 | N | ASN | B | 364 | -23.279 | 63.075 | 21.361 | 1.00 | 33.51 | 7 |
| | ATOM | 777 | CA | ASN | B | 364 | -24.683 | 62.701 | 21.377 | 1.00 | 38.03 | 6 |
| | ATOM | 778 | CB | ASN | B | 364 | -24.855 | 61.369 | 22.111 | 1.00 | 42.32 | 6 |
| 35 | ATOM | 779 | CG | ASN | B | 364 | -24.008 | 60.271 | 21.524 | 1.00 | 53.11 | 6 |
| | ATOM | 780 | OD1 | ASN | B | 364 | -24.183 | 59.895 | 20.344 | 1.00 | 59.51 | 8 |
| | ATOM | 781 | ND2 | ASN | B | 364 | -23.102 | 59.746 | 22.325 | 1.00 | 55.95 | 7 |
| | ATOM | 782 | C | ASN | B | 364 | -25.494 | 63.771 | 22.091 | 1.00 | 31.89 | 6 |
| | ATOM | 783 | O | ASN | B | 364 | -26.279 | 63.471 | 22.990 | 1.00 | 30.28 | 8 |
| 40 | ATOM | 784 | N | LEU | B | 365 | -25.306 | 65.018 | 21.673 | 1.00 | 27.62 | 7 |
| | ATOM | 785 | CA | LEU | B | 365 | -26.005 | 66.144 | 22.280 | 1.00 | 29.36 | 6 |
| | ATOM | 786 | CB | LEU | B | 365 | -25.402 | 67.443 | 21.743 | 1.00 | 27.54 | 6 |
| | ATOM | 787 | CG | LEU | B | 365 | -23.897 | 67.453 | 21.738 | 1.00 | 38.91 | 6 |
| | ATOM | 788 | CD1 | LEU | B | 365 | -23.391 | 68.766 | 21.190 | 1.00 | 34.47 | 6 |
| 45 | ATOM | 789 | CD2 | LEU | B | 365 | -23.393 | 67.214 | 23.143 | 1.00 | 34.24 | 6 |
| | ATOM | 790 | C | LEU | B | 365 | -27.496 | 66.074 | 21.987 | 1.00 | 26.23 | 6 |
| | ATOM | 791 | O | LEU | B | 365 | -27.911 | 65.790 | 20.863 | 1.00 | 27.06 | 8 |
| | ATOM | 792 | N | ASP | B | 366 | -28.296 | 66.321 | 23.022 | 1.00 | 25.23 | 7 |
| | ATOM | 793 | CA | ASP | B | 366 | -29.752 | 66.320 | 22.878 | 1.00 | 26.07 | 6 |
| 50 | ATOM | 794 | CB | ASP | B | 366 | -30.441 | 65.651 | 24.076 | 1.00 | 29.68 | 6 |
| | ATOM | 795 | CG | ASP | B | 366 | -30.221 | 66.374 | 25.360 | 1.00 | 35.74 | 6 |
| | ATOM | 796 | OD1 | ASP | B | 366 | -30.277 | 67.617 | 25.387 | 1.00 | 36.78 | 8 |
| | ATOM | 797 | OD2 | ASP | B | 366 | -30.017 | 65.711 | 26.410 | 1.00 | 41.23 | 8 |
| | ATOM | 798 | C | ASP | B | 366 | -30.230 | 67.752 | 22.740 | 1.00 | 27.70 | 6 |
| 55 | ATOM | 799 | O | ASP | B | 366 | -29.552 | 68.678 | 23.171 | 1.00 | 31.94 | 8 |
| | ATOM | 800 | N | ASP | B | 367 | -31.409 | 67.913 | 22.142 | 1.00 | 29.18 | 7 |
| | ATOM | 801 | CA | ASP | B | 367 | -32.031 | 69.225 | 21.930 | 1.00 | 32.72 | 6 |
| | ATOM | 802 | CB | ASP | B | 367 | -33.558 | 69.106 | 22.071 | 1.00 | 38.04 | 6 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 803 | CG | ASP | B | 367 | -34.172 | 68.166 | 21.081 | 1.00 | 42.43 | 6 |
| | ATOM | 804 | OD1 | ASP | B | 367 | -34.051 | 68.373 | 19.854 | 1.00 | 35.95 | 8 |
| | ATOM | 805 | OD2 | ASP | B | 367 | -34.829 | 67.188 | 21.504 | 1.00 | 51.42 | 8 |
| | ATOM | 806 | C | ASP | B | 367 | -31.496 | 70.238 | 22.959 | 1.00 | 33.71 | 6 |
| | ATOM | 807 | O | ASP | B | 367 | -30.791 | 71.188 | 22.624 | 1.00 | 38.30 | 8 |
| 10 | ATOM | 808 | N | THR | B | 368 | -31.858 | 69.997 | 24.218 | 1.00 | 31.06 | 7 |
| | ATOM | 809 | CA | THR | B | 368 | -31.453 | 70.822 | 25.344 | 1.00 | 26.28 | 6 |
| | ATOM | 810 | CB | THR | B | 368 | -31.567 | 70.020 | 26.643 | 1.00 | 27.30 | 6 |
| | ATOM | 811 | OG1 | THR | B | 368 | -32.916 | 69.578 | 26.824 | 1.00 | 33.42 | 8 |
| | ATOM | 812 | CG2 | THR | B | 368 | -31.143 | 70.855 | 27.824 | 1.00 | 25.16 | 6 |
| 15 | ATOM | 813 | C | THR | B | 368 | -30.025 | 71.315 | 25.181 | 1.00 | 21.13 | 6 |
| | ATOM | 814 | O | THR | B | 368 | -29.746 | 72.508 | 25.150 | 1.00 | 23.17 | 8 |
| | ATOM | 815 | N | GLU | B | 369 | -29.123 | 70.354 | 25.072 | 1.00 | 21.32 | 7 |
| | ATOM | 816 | CA | GLU | B | 369 | -27.711 | 70.634 | 24.932 | 1.00 | 28.00 | 6 |
| | ATOM | 817 | CB | GLU | B | 369 | -26.947 | 69.306 | 24.878 | 1.00 | 32.79 | 6 |
| 20 | ATOM | 818 | CG | GLU | B | 369 | -27.229 | 68.433 | 26.130 | 1.00 | 36.29 | 6 |
| | ATOM | 819 | CD | GLU | B | 369 | -26.689 | 67.051 | 26.083 | 1.00 | 41.03 | 6 |
| | ATOM | 820 | OE1 | GLU | B | 369 | -26.960 | 66.318 | 25.102 | 1.00 | 42.05 | 8 |
| | ATOM | 821 | OE2 | GLU | B | 369 | -25.992 | 66.645 | 27.048 | 1.00 | 42.03 | 8 |
| | ATOM | 822 | C | GLU | B | 369 | -27.428 | 71.527 | 23.731 | 1.00 | 25.57 | 6 |
| 25 | ATOM | 823 | O | GLU | B | 369 | -26.780 | 72.549 | 23.886 | 1.00 | 20.56 | 8 |
| | ATOM | 824 | N | VAL | B | 370 | -27.922 | 71.154 | 22.548 | 1.00 | 25.39 | 7 |
| | ATOM | 825 | CA | VAL | B | 370 | -27.710 | 71.968 | 21.355 | 1.00 | 25.99 | 6 |
| | ATOM | 826 | CB | VAL | B | 370 | -28.457 | 71.429 | 20.130 | 1.00 | 26.15 | 6 |
| | ATOM | 827 | CG1 | VAL | B | 370 | -28.255 | 72.358 | 18.953 | 1.00 | 27.65 | 6 |
| 30 | ATOM | 828 | CG2 | VAL | B | 370 | -28.014 | 70.021 | 19.788 | 1.00 | 17.70 | 6 |
| | ATOM | 829 | C | VAL | B | 370 | -28.238 | 73.346 | 21.676 | 1.00 | 26.49 | 6 |
| | ATOM | 830 | O | VAL | B | 370 | -27.580 | 74.351 | 21.445 | 1.00 | 28.16 | 8 |
| | ATOM | 831 | N | ALA | B | 371 | -29.450 | 73.362 | 22.213 | 1.00 | 21.01 | 7 |
| | ATOM | 832 | CA | ALA | B | 371 | -30.145 | 74.589 | 22.573 | 1.00 | 19.57 | 6 |
| 35 | ATOM | 833 | CB | ALA | B | 371 | -31.414 | 74.246 | 23.335 | 1.00 | 18.62 | 6 |
| | ATOM | 834 | C | ALA | B | 371 | -29.256 | 75.501 | 23.401 | 1.00 | 23.48 | 6 |
| | ATOM | 835 | O | ALA | B | 371 | -28.936 | 76.613 | 22.989 | 1.00 | 32.67 | 8 |
| | ATOM | 836 | N | LEU | B | 372 | -28.860 | 75.008 | 24.571 | 1.00 | 22.89 | 7 |
| | ATOM | 837 | CA | LEU | B | 372 | -27.999 | 75.758 | 25.472 | 1.00 | 23.28 | 6 |
| 40 | ATOM | 838 | CB | LEU | B | 372 | -27.606 | 74.860 | 26.658 | 1.00 | 27.76 | 6 |
| | ATOM | 839 | CG | LEU | B | 372 | -28.728 | 74.524 | 27.619 | 1.00 | 21.18 | 6 |
| | ATOM | 840 | CD1 | LEU | B | 372 | -28.272 | 73.529 | 28.648 | 1.00 | 27.64 | 6 |
| | ATOM | 841 | CD2 | LEU | B | 372 | -29.198 | 75.801 | 28.284 | 1.00 | 20.90 | 6 |
| | ATOM | 842 | C | LEU | B | 372 | -26.769 | 76.268 | 24.722 | 1.00 | 21.34 | 6 |
| 45 | ATOM | 843 | O | LEU | B | 372 | -26.439 | 77.454 | 24.762 | 1.00 | 23.16 | 8 |
| | ATOM | 844 | N | LEU | B | 373 | -26.111 | 75.349 | 24.023 | 1.00 | 24.42 | 7 |
| | ATOM | 845 | CA | LEU | B | 373 | -24.916 | 75.669 | 23.254 | 1.00 | 23.78 | 6 |
| | ATOM | 846 | CB | LEU | B | 373 | -24.525 | 74.446 | 22.396 | 1.00 | 22.18 | 6 |
| | ATOM | 847 | CG | LEU | B | 373 | -23.098 | 74.283 | 21.942 | 1.00 | 31.52 | 6 |
| 50 | ATOM | 848 | CD1 | LEU | B | 373 | -22.196 | 74.576 | 23.100 | 1.00 | 31.93 | 6 |
| | ATOM | 849 | CD2 | LEU | B | 373 | -22.873 | 72.889 | 21.457 | 1.00 | 30.24 | 6 |
| | ATOM | 850 | C | LEU | B | 373 | -25.235 | 76.902 | 22.405 | 1.00 | 25.69 | 6 |
| | ATOM | 851 | O | LEU | B | 373 | -24.491 | 77.880 | 22.416 | 1.00 | 30.13 | 8 |
| | ATOM | 852 | N | GLN | B | 374 | -26.368 | 76.842 | 21.707 | 1.00 | 26.24 | 7 |
| 55 | ATOM | 853 | CA | GLN | B | 374 | -26.836 | 77.922 | 20.839 | 1.00 | 21.60 | 6 |
| | ATOM | 854 | CB | GLN | B | 374 | -28.196 | 77.571 | 20.221 | 1.00 | 24.57 | 6 |
| | ATOM | 855 | CG | GLN | B | 374 | -28.188 | 76.330 | 19.348 | 1.00 | 21.02 | 6 |
| | ATOM | 856 | CD | GLN | B | 374 | -29.538 | 76.071 | 18.698 | 1.00 | 22.86 | 6 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 857 | OE1 | GLN | B | 374 | -29.720 | 75.049 | 18.009 | 1.00 | 24.07 | 8 |
| | ATOM | 858 | NE2 | GLN | B | 374 | -30.473 | 76.980 | 18.901 | 1.00 | 25.59 | 7 |
| | ATOM | 859 | C | GLN | B | 374 | -26.988 | 79.249 | 21.569 | 1.00 | 20.66 | 6 |
| | ATOM | 860 | O | GLN | B | 374 | -26.733 | 80.307 | 20.994 | 1.00 | 24.47 | 8 |
| | ATOM | 861 | N | ALA | B | 375 | -27.429 | 79.182 | 22.825 | 1.00 | 16.26 | 7 |
| 10 | ATOM | 862 | CA | ALA | B | 375 | -27.639 | 80.374 | 23.631 | 1.00 | 17.16 | 6 |
| | ATOM | 863 | CB | ALA | B | 375 | -28.435 | 80.025 | 24.865 | 1.00 | 19.53 | 6 |
| | ATOM | 864 | C | ALA | B | 375 | -26.304 | 80.966 | 24.025 | 1.00 | 25.13 | 6 |
| | ATOM | 865 | O | ALA | B | 375 | -26.074 | 82.154 | 23.833 | 1.00 | 23.81 | 8 |
| | ATOM | 866 | N | VAL | B | 376 | -25.433 | 80.111 | 24.568 | 1.00 | 24.57 | 7 |
| 15 | ATOM | 867 | CA | VAL | B | 376 | -24.102 | 80.526 | 24.986 | 1.00 | 25.80 | 6 |
| | ATOM | 868 | CB | VAL | B | 376 | -23.192 | 79.321 | 25.234 | 1.00 | 26.48 | 6 |
| | ATOM | 869 | CG1 | VAL | B | 376 | -21.806 | 79.780 | 25.620 | 1.00 | 23.20 | 6 |
| | ATOM | 870 | CG2 | VAL | B | 376 | -23.771 | 78.433 | 26.310 | 1.00 | 19.08 | 6 |
| | ATOM | 871 | C | VAL | B | 376 | -23.510 | 81.403 | 23.898 | 1.00 | 25.69 | 6 |
| 20 | ATOM | 872 | O | VAL | B | 376 | -22.796 | 82.364 | 24.166 | 1.00 | 27.87 | 8 |
| | ATOM | 873 | N | LEU | B | 377 | -23.827 | 81.049 | 22.659 | 1.00 | 23.09 | 7 |
| | ATOM | 874 | CA | LEU | B | 377 | -23.340 | 81.774 | 21.492 | 1.00 | 22.86 | 6 |
| | ATOM | 875 | CB | LEU | B | 377 | -23.552 | 80.920 | 20.230 | 1.00 | 18.50 | 6 |
| | ATOM | 876 | CG | LEU | B | 377 | -22.756 | 79.638 | 20.146 | 1.00 | 22.65 | 6 |
| 25 | ATOM | 877 | CD1 | LEU | B | 377 | -23.221 | 78.786 | 19.000 | 1.00 | 16.70 | 6 |
| | ATOM | 878 | CD2 | LEU | B | 377 | -21.300 | 79.995 | 20.000 | 1.00 | 19.58 | 6 |
| | ATOM | 879 | C | LEU | B | 377 | -24.073 | 83.102 | 21.384 | 1.00 | 26.14 | 6 |
| | ATOM | 880 | O | LEU | B | 377 | -23.464 | 84.164 | 21.419 | 1.00 | 20.62 | 8 |
| | ATOM | 881 | N | LEU | B | 378 | -25.396 | 83.023 | 21.265 | 1.00 | 28.99 | 7 |
| 30 | ATOM | 882 | CA | LEU | B | 378 | -26.228 | 84.217 | 21.147 | 1.00 | 28.87 | 6 |
| | ATOM | 883 | CB | LEU | B | 378 | -27.696 | 83.894 | 21.450 | 1.00 | 26.89 | 6 |
| | ATOM | 884 | CG | LEU | B | 378 | -28.648 | 85.068 | 21.500 | 1.00 | 28.83 | 6 |
| | ATOM | 885 | CD1 | LEU | B | 378 | -28.507 | 85.854 | 20.225 | 1.00 | 27.97 | 6 |
| | ATOM | 886 | CD2 | LEU | B | 378 | -30.072 | 84.605 | 21.692 | 1.00 | 27.69 | 6 |
| 35 | ATOM | 887 | C | LEU | B | 378 | -25.738 | 85.280 | 22.090 | 1.00 | 31.09 | 6 |
| | ATOM | 888 | O | LEU | B | 378 | -25.398 | 86.379 | 21.651 | 1.00 | 31.77 | 8 |
| | ATOM | 889 | N | MET | B | 379 | -25.695 | 84.931 | 23.376 | 1.00 | 31.44 | 7 |
| | ATOM | 890 | CA | MET | B | 379 | -25.291 | 85.851 | 24.434 | 1.00 | 32.62 | 6 |
| | ATOM | 891 | CB | MET | B | 379 | -25.797 | 85.335 | 25.793 | 1.00 | 31.45 | 6 |
| 40 | ATOM | 892 | CG | MET | B | 379 | -27.332 | 85.262 | 25.883 | 1.00 | 38.75 | 6 |
| | ATOM | 893 | SD | MET | B | 379 | -28.020 | 86.915 | 25.550 | 1.00 | 41.27 | 16 |
| | ATOM | 894 | CE | MET | B | 379 | -29.814 | 86.586 | 25.513 | 1.00 | 35.68 | 6 |
| | ATOM | 895 | C | MET | B | 379 | -23.796 | 86.129 | 24.538 | 1.00 | 33.72 | 6 |
| | ATOM | 896 | O | MET | B | 379 | -23.246 | 86.190 | 25.633 | 1.00 | 36.29 | 8 |
| 45 | ATOM | 897 | N | SER | B | 380 | -23.152 | 86.335 | 23.399 | 1.00 | 34.49 | 7 |
| | ATOM | 898 | CA | SER | B | 380 | -21.738 | 86.659 | 23.391 | 1.00 | 33.97 | 6 |
| | ATOM | 899 | CB | SER | B | 380 | -21.132 | 86.360 | 22.010 | 1.00 | 31.24 | 6 |
| | ATOM | 900 | OG | SER | B | 380 | -21.224 | 84.978 | 21.696 | 1.00 | 39.42 | 8 |
| | ATOM | 901 | C | SER | B | 380 | -21.635 | 88.145 | 23.705 | 1.00 | 39.69 | 6 |
| 50 | ATOM | 902 | O | SER | B | 380 | -22.084 | 88.989 | 22.933 | 1.00 | 44.64 | 8 |
| | ATOM | 903 | N | SER | B | 381 | -21.053 | 88.451 | 24.857 | 1.00 | 41.04 | 7 |
| | ATOM | 904 | CA | SER | B | 381 | -20.907 | 89.826 | 25.308 | 1.00 | 44.91 | 6 |
| | ATOM | 905 | CB | SER | B | 381 | -20.610 | 89.832 | 26.797 | 1.00 | 44.50 | 6 |
| | ATOM | 906 | OG | SER | B | 381 | -19.351 | 89.229 | 27.037 | 1.00 | 45.42 | 8 |
| 55 | ATOM | 907 | C | SER | B | 381 | -19.815 | 90.614 | 24.602 | 1.00 | 44.59 | 6 |
| | ATOM | 908 | O | SER | B | 381 | -19.725 | 91.825 | 24.751 | 1.00 | 49.32 | 8 |
| | ATOM | 909 | N | ASP | B | 382 | -18.977 | 89.922 | 23.848 | 1.00 | 43.75 | 7 |
| | ATOM | 910 | CA | ASP | B | 382 | -17.886 | 90.556 | 23.144 | 1.00 | 43.93 | 6 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 911 | CB | ASP | B | 382 | -16.727 | 89.562 | 23.028 | 1.00 | 48.39 | 6 |
| | ATOM | 912 | CG | ASP | B | 382 | -17.142 | 88.232 | 22.471 | 1.00 | 53.23 | 6 |
| | ATOM | 913 | OD1 | ASP | B | 382 | -18.102 | 87.621 | 23.002 | 1.00 | 56.97 | 8 |
| | ATOM | 914 | OD2 | ASP | B | 382 | -16.513 | 87.753 | 21.480 | 1.00 | 58.91 | 8 |
| | ATOM | 915 | C | ASP | B | 382 | -18.191 | 91.172 | 21.772 | 1.00 | 41.09 | 6 |
| 10 | ATOM | 916 | O | ASP | B | 382 | -17.366 | 91.899 | 21.229 | 1.00 | 40.93 | 8 |
| | ATOM | 917 | N | ARG | B | 383 | -19.369 | 90.908 | 21.224 | 1.00 | 42.63 | 7 |
| | ATOM | 918 | CA | ARG | B | 383 | -19.698 | 91.445 | 19.934 | 1.00 | 43.32 | 6 |
| | ATOM | 919 | CB | ARG | B | 383 | -21.131 | 91.101 | 19.557 | 1.00 | 42.31 | 6 |
| | ATOM | 920 | CG | ARG | B | 383 | -21.619 | 89.672 | 19.811 | 1.00 | 40.83 | 6 |
| 15 | ATOM | 921 | CD | ARG | B | 383 | -21.144 | 88.627 | 18.804 | 1.00 | 38.09 | 6 |
| | ATOM | 922 | NE | ARG | B | 383 | -21.922 | 87.415 | 18.943 | 1.00 | 37.33 | 7 |
| | ATOM | 923 | CZ | ARG | B | 383 | -21.584 | 86.250 | 18.411 | 1.00 | 38.35 | 6 |
| | ATOM | 924 | NH1 | ARG | B | 383 | -20.465 | 86.143 | 17.700 | 1.00 | 33.70 | 7 |
| | ATOM | 925 | NH2 | ARG | B | 383 | -22.369 | 85.196 | 18.604 | 1.00 | 35.46 | 7 |
| 20 | ATOM | 926 | C | ARG | B | 383 | -19.591 | 92.958 | 20.007 | 1.00 | 44.96 | 6 |
| | ATOM | 927 | O | ARG | B | 383 | -20.050 | 93.577 | 20.980 | 1.00 | 45.60 | 8 |
| | ATOM | 928 | N | PRO | B | 384 | -18.975 | 93.579 | 19.005 | 1.00 | 45.33 | 7 |
| | ATOM | 929 | CD | PRO | B | 384 | -18.395 | 92.881 | 17.854 | 1.00 | 46.85 | 6 |
| | ATOM | 930 | CA | PRO | B | 384 | -18.808 | 95.035 | 18.947 | 1.00 | 47.37 | 6 |
| 25 | ATOM | 931 | CB | PRO | B | 384 | -17.868 | 95.255 | 17.764 | 1.00 | 46.90 | 6 |
| | ATOM | 932 | CG | PRO | B | 384 | -17.575 | 93.934 | 17.187 | 1.00 | 46.41 | 6 |
| | ATOM | 933 | C | PRO | B | 384 | -20.125 | 95.778 | 18.762 | 1.00 | 48.29 | 6 |
| | ATOM | 934 | O | PRO | B | 384 | -21.048 | 95.277 | 18.120 | 1.00 | 48.34 | 8 |
| | ATOM | 935 | N | GLY | B | 385 | -20.185 | 96.994 | 19.314 | 1.00 | 49.88 | 7 |
| 30 | ATOM | 936 | CA | GLY | B | 385 | -21.371 | 97.838 | 19.192 | 1.00 | 50.35 | 6 |
| | ATOM | 937 | C | GLY | B | 385 | -22.410 | 97.615 | 20.265 | 1.00 | 50.70 | 6 |
| | ATOM | 938 | O | GLY | B | 385 | -23.382 | 98.363 | 20.374 | 1.00 | 53.48 | 8 |
| | ATOM | 939 | N | LEU | B | 386 | -22.205 | 96.557 | 21.044 | 1.00 | 49.04 | 7 |
| | ATOM | 940 | CA | LEU | B | 386 | -23.136 | 96.211 | 22.101 | 1.00 | 50.53 | 6 |
| 35 | ATOM | 941 | CB | LEU | B | 386 | -22.640 | 94.972 | 22.853 | 1.00 | 45.17 | 6 |
| | ATOM | 942 | CG | LEU | B | 386 | -22.744 | 93.653 | 22.121 | 1.00 | 48.26 | 6 |
| | ATOM | 943 | CD1 | LEU | B | 386 | -22.122 | 92.525 | 22.938 | 1.00 | 41.68 | 6 |
| | ATOM | 944 | CD2 | LEU | B | 386 | -24.215 | 93.376 | 21.852 | 1.00 | 38.40 | 6 |
| | ATOM | 945 | C | LEU | B | 386 | -23.322 | 97.357 | 23.058 | 1.00 | 52.13 | 6 |
| 40 | ATOM | 946 | O | LEU | B | 386 | -22.438 | 98.182 | 23.234 | 1.00 | 53.67 | 8 |
| | ATOM | 947 | N | ALA | B | 387 | -24.499 | 97.398 | 23.666 | 1.00 | 53.42 | 7 |
| | ATOM | 948 | CA | ALA | B | 387 | -24.830 | 98.441 | 24.624 | 1.00 | 56.01 | 6 |
| | ATOM | 949 | CB | ALA | B | 387 | -26.223 | 98.993 | 24.339 | 1.00 | 56.47 | 6 |
| | ATOM | 950 | C | ALA | B | 387 | -24.775 | 97.853 | 26.024 | 1.00 | 55.52 | 6 |
| 45 | ATOM | 951 | O | ALA | B | 387 | -23.798 | 98.027 | 26.753 | 1.00 | 53.75 | 8 |
| | ATOM | 952 | N | CYS | B | 388 | -25.843 | 97.145 | 26.371 | 1.00 | 56.03 | 7 |
| | ATOM | 953 | CA | CYS | B | 388 | -26.000 | 96.525 | 27.673 | 1.00 | 59.57 | 6 |
| | ATOM | 954 | CB | CYS | B | 388 | -27.469 | 96.134 | 27.839 | 1.00 | 59.23 | 6 |
| | ATOM | 955 | SG | CYS | B | 388 | -28.620 | 97.392 | 27.264 | 1.00 | 58.64 | 16 |
| 50 | ATOM | 956 | C | CYS | B | 388 | -25.105 | 95.283 | 27.798 | 1.00 | 62.18 | 6 |
| | ATOM | 957 | O | CYS | B | 388 | -25.590 | 94.164 | 27.868 | 1.00 | 67.88 | 8 |
| | ATOM | 958 | N | VAL | B | 389 | -23.789 | 95.510 | 27.824 | 1.00 | 60.78 | 7 |
| | ATOM | 959 | CA | VAL | B | 389 | -22.797 | 94.434 | 27.959 | 1.00 | 57.70 | 6 |
| | ATOM | 960 | CB | VAL | B | 389 | -21.355 | 94.976 | 27.998 | 1.00 | 57.09 | 6 |
| 55 | ATOM | 961 | CG1 | VAL | B | 389 | -20.361 | 93.832 | 28.085 | 1.00 | 59.03 | 6 |
| | ATOM | 962 | CG2 | VAL | B | 389 | -21.065 | 95.845 | 26.791 | 1.00 | 53.98 | 6 |
| | ATOM | 963 | C | VAL | B | 389 | -23.078 | 93.642 | 29.230 | 1.00 | 57.77 | 6 |
| | ATOM | 964 | O | VAL | B | 389 | -23.727 | 92.602 | 29.203 | 1.00 | 60.94 | 8 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 965 | N | ALA | B | 390 | -22.561 | 94.159 | 30.332 | 1.00 | 52.68 | 7 |
| | ATOM | 966 | CA | ALA | B | 390 | -22.684 | 93.570 | 31.659 | 1.00 | 48.41 | 6 |
| | ATOM | 967 | CB | ALA | B | 390 | -22.650 | 94.681 | 32.716 | 1.00 | 45.19 | 6 |
| | ATOM | 968 | C | ALA | B | 390 | -23.905 | 92.697 | 31.877 | 1.00 | 47.63 | 6 |
| | ATOM | 969 | O | ALA | B | 390 | -23.784 | 91.576 | 32.369 | 1.00 | 51.95 | 8 |
| 10 | ATOM | 970 | N | ARG | B | 391 | -25.075 | 93.216 | 31.498 | 1.00 | 47.11 | 7 |
| | ATOM | 971 | CA | ARG | B | 391 | -26.330 | 92.481 | 31.656 | 1.00 | 51.64 | 6 |
| | ATOM | 972 | CB | ARG | B | 391 | -27.502 | 93.318 | 31.122 | 1.00 | 54.22 | 6 |
| | ATOM | 973 | CG | ARG | B | 391 | -28.887 | 92.713 | 31.430 | 1.00 | 64.20 | 6 |
| | ATOM | 974 | CD | ARG | B | 391 | -30.059 | 93.582 | 30.929 | 1.00 | 73.80 | 6 |
| 15 | ATOM | 975 | NE | ARG | B | 391 | -31.361 | 93.097 | 31.378 | 1.00 | 79.76 | 7 |
| | ATOM | 976 | CZ | ARG | B | 391 | -31.736 | 93.015 | 32.656 | 1.00 | 84.27 | 6 |
| | ATOM | 977 | NH1 | ARG | B | 391 | -30.887 | 93.372 | 33.625 | 1.00 | 85.28 | 7 |
| | ATOM | 978 | NH2 | ARG | B | 391 | -32.957 | 92.566 | 32.955 | 1.00 | 86.84 | 7 |
| | ATOM | 979 | C | ARG | B | 391 | -26.277 | 91.133 | 30.940 | 1.00 | 48.18 | 6 |
| 20 | ATOM | 980 | O | ARG | B | 391 | -26.724 | 90.119 | 31.465 | 1.00 | 49.57 | 8 |
| | ATOM | 981 | N | ILE | B | 392 | -25.743 | 91.167 | 29.718 | 1.00 | 45.01 | 7 |
| | ATOM | 982 | CA | ILE | B | 392 | -25.592 | 89.999 | 28.867 | 1.00 | 48.77 | 6 |
| | ATOM | 983 | CB | ILE | B | 392 | -25.112 | 90.424 | 27.469 | 1.00 | 46.45 | 6 |
| | ATOM | 984 | CG2 | ILE | B | 392 | -24.805 | 89.221 | 26.614 | 1.00 | 42.35 | 6 |
| 25 | ATOM | 985 | CG1 | ILE | B | 392 | -26.178 | 91.283 | 26.768 | 1.00 | 49.69 | 6 |
| | ATOM | 986 | CD1 | ILE | B | 392 | -25.762 | 91.768 | 25.386 | 1.00 | 51.09 | 6 |
| | ATOM | 987 | C | ILE | B | 392 | -24.671 | 88.935 | 29.462 | 1.00 | 50.90 | 6 |
| | ATOM | 988 | O | ILE | B | 392 | -25.086 | 87.780 | 29.605 | 1.00 | 52.21 | 8 |
| | ATOM | 989 | N | GLU | B | 393 | -23.431 | 89.298 | 29.790 | 1.00 | 50.43 | 7 |
| 30 | ATOM | 990 | CA | GLU | B | 393 | -22.504 | 88.328 | 30.378 | 1.00 | 50.30 | 6 |
| | ATOM | 991 | CB | GLU | B | 393 | -21.314 | 89.022 | 31.044 | 1.00 | 53.97 | 6 |
| | ATOM | 992 | CG | GLU | B | 393 | -20.063 | 89.005 | 30.209 | 1.00 | 62.18 | 6 |
| | ATOM | 993 | CD | GLU | B | 393 | -18.877 | 89.415 | 30.976 | 1.00 | 67.69 | 6 |
| | ATOM | 994 | OE1 | GLU | B | 393 | -17.709 | 89.264 | 30.656 | 1.00 | 66.42 | 8 |
| 35 | ATOM | 995 | OE2 | GLU | B | 393 | -18.897 | 89.976 | 32.052 | 1.00 | 70.64 | 8 |
| | ATOM | 996 | C | GLU | B | 393 | -23.251 | 87.477 | 31.416 | 1.00 | 49.31 | 6 |
| | ATOM | 997 | O | GLU | B | 393 | -23.226 | 86.260 | 31.303 | 1.00 | 49.53 | 8 |
| | ATOM | 998 | N | LYS | B | 394 | -23.898 | 88.153 | 32.409 | 1.00 | 46.07 | 7 |
| | ATOM | 999 | CA | LYS | B | 394 | -24.721 | 87.579 | 33.506 | 1.00 | 45.76 | 6 |
| 40 | ATOM | 1000 | CB | LYS | B | 394 | -25.594 | 88.693 | 34.161 | 1.00 | 43.85 | 6 |
| | ATOM | 1001 | C | LYS | B | 394 | -25.626 | 86.548 | 32.851 | 1.00 | 46.69 | 6 |
| | ATOM | 1002 | O | LYS | B | 394 | -25.772 | 85.430 | 33.329 | 1.00 | 49.13 | 8 |
| | ATOM | 1003 | N | TYR | B | 395 | -26.203 | 86.948 | 31.719 | 1.00 | 46.57 | 7 |
| | ATOM | 1004 | CA | TYR | B | 395 | -27.076 | 86.078 | 30.938 | 1.00 | 43.33 | 6 |
| 45 | ATOM | 1005 | CB | TYR | B | 395 | -27.621 | 86.821 | 29.716 | 1.00 | 48.44 | 6 |
| | ATOM | 1006 | CG | TYR | B | 395 | -28.827 | 87.688 | 29.980 | 1.00 | 53.83 | 6 |
| | ATOM | 1007 | CD1 | TYR | B | 395 | -29.204 | 88.680 | 29.080 | 1.00 | 56.43 | 6 |
| | ATOM | 1008 | CE1 | TYR | B | 395 | -30.331 | 89.469 | 29.309 | 1.00 | 59.73 | 6 |
| | ATOM | 1009 | CD2 | TYR | B | 395 | -29.596 | 87.509 | 31.113 | 1.00 | 56.47 | 6 |
| 50 | ATOM | 1010 | CE2 | TYR | B | 395 | -30.723 | 88.295 | 31.346 | 1.00 | 62.60 | 6 |
| | ATOM | 1011 | CZ | TYR | B | 395 | -31.090 | 89.281 | 30.446 | 1.00 | 63.18 | 6 |
| | ATOM | 1012 | OH | TYR | B | 395 | -32.189 | 90.068 | 30.671 | 1.00 | 64.46 | 8 |
| | ATOM | 1013 | C | TYR | B | 395 | -26.276 | 84.867 | 30.485 | 1.00 | 37.30 | 6 |
| | ATOM | 1014 | O | TYR | B | 395 | -26.611 | 83.737 | 30.825 | 1.00 | 34.10 | 8 |
| 55 | ATOM | 1015 | N | GLN | B | 396 | -25.213 | 85.108 | 29.718 | 1.00 | 31.92 | 7 |
| | ATOM | 1016 | CA | GLN | B | 396 | -24.380 | 84.018 | 29.244 | 1.00 | 34.81 | 6 |
| | ATOM | 1017 | CB | GLN | B | 396 | -23.176 | 84.550 | 28.464 | 1.00 | 32.64 | 6 |
| | ATOM | 1018 | CG | GLN | B | 396 | -22.184 | 83.470 | 28.103 | 1.00 | 29.57 | 6 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 1019 | CD | GLN | B | 396 | -21.214 | 83.871 | 27.016 | 1.00 | 29.46 | 6 |
| | ATOM | 1020 | OE1 | GLN | B | 396 | -20.547 | 84.930 | 27.109 | 1.00 | 34.65 | 8 |
| | ATOM | 1021 | NE2 | GLN | B | 396 | -21.112 | 83.032 | 25.992 | 1.00 | 27.21 | 7 |
| | ATOM | 1022 | C | GLN | B | 396 | -23.908 | 83.207 | 30.434 | 1.00 | 37.13 | 6 |
| | ATOM | 1023 | O | GLN | B | 396 | -23.876 | 81.986 | 30.384 | 1.00 | 37.36 | 8 |
| 10 | ATOM | 1024 | N | ASP | B | 397 | -23.544 | 83.903 | 31.508 | 1.00 | 38.61 | 7 |
| | ATOM | 1025 | CA | ASP | B | 397 | -23.069 | 83.250 | 32.717 | 1.00 | 40.37 | 6 |
| | ATOM | 1026 | CB | ASP | B | 397 | -22.617 | 84.297 | 33.754 | 1.00 | 40.51 | 6 |
| | ATOM | 1027 | CG | ASP | B | 397 | -21.360 | 85.025 | 33.352 | 1.00 | 43.77 | 6 |
| | ATOM | 1028 | OD1 | ASP | B | 397 | -20.337 | 84.366 | 33.054 | 1.00 | 46.50 | 8 |
| 15 | ATOM | 1029 | OD2 | ASP | B | 397 | -21.343 | 86.287 | 33.350 | 1.00 | 51.34 | 8 |
| | ATOM | 1030 | C | ASP | B | 397 | -24.223 | 82.422 | 33.267 | 1.00 | 38.62 | 6 |
| | ATOM | 1031 | O | ASP | B | 397 | -24.023 | 81.327 | 33.778 | 1.00 | 39.20 | 8 |
| | ATOM | 1032 | N | SER | B | 398 | -25.432 | 82.962 | 33.138 | 1.00 | 37.84 | 7 |
| | ATOM | 1033 | CA | SER | B | 398 | -26.633 | 82.293 | 33.622 | 1.00 | 37.80 | 6 |
| 20 | ATOM | 1034 | CB | SER | B | 398 | -27.830 | 83.246 | 33.501 | 1.00 | 34.28 | 6 |
| | ATOM | 1035 | OG | SER | B | 398 | -28.995 | 82.715 | 34.114 | 1.00 | 46.60 | 8 |
| | ATOM | 1036 | C | SER | B | 398 | -26.911 | 80.997 | 32.867 | 1.00 | 38.41 | 6 |
| | ATOM | 1037 | O | SER | B | 398 | -27.454 | 80.047 | 33.433 | 1.00 | 39.98 | 8 |
| | ATOM | 1038 | N | PHE | B | 399 | -26.546 | 80.963 | 31.587 | 1.00 | 34.82 | 7 |
| 25 | ATOM | 1039 | CA | PHE | B | 399 | -26.772 | 79.768 | 30.781 | 1.00 | 35.96 | 6 |
| | ATOM | 1040 | CB | PHE | B | 399 | -26.892 | 80.100 | 29.293 | 1.00 | 35.75 | 6 |
| | ATOM | 1041 | CG | PHE | B | 399 | -28.211 | 80.717 | 28.906 | 1.00 | 39.30 | 6 |
| | ATOM | 1042 | CD1 | PHE | B | 399 | -28.466 | 82.056 | 29.109 | 1.00 | 39.86 | 6 |
| | ATOM | 1043 | CD2 | PHE | B | 399 | -29.194 | 79.938 | 28.355 | 1.00 | 36.81 | 6 |
| 30 | ATOM | 1044 | CE1 | PHE | B | 399 | -29.700 | 82.602 | 28.739 | 1.00 | 41.25 | 6 |
| | ATOM | 1045 | CE2 | PHE | B | 399 | -30.424 | 80.483 | 27.987 | 1.00 | 43.61 | 6 |
| | ATOM | 1046 | CZ | PHE | B | 399 | -30.677 | 81.813 | 28.181 | 1.00 | 40.34 | 6 |
| | ATOM | 1047 | C | PHE | B | 399 | -25.658 | 78.754 | 30.976 | 1.00 | 33.48 | 6 |
| | ATOM | 1048 | O | PHE | B | 399 | -25.927 | 77.589 | 31.256 | 1.00 | 26.86 | 8 |
| 35 | ATOM | 1049 | N | LEU | B | 400 | -24.408 | 79.187 | 30.796 | 1.00 | 31.47 | 7 |
| | ATOM | 1050 | CA | LEU | B | 400 | -23.275 | 78.291 | 30.945 | 1.00 | 37.41 | 6 |
| | ATOM | 1051 | CB | LEU | B | 400 | -21.976 | 79.091 | 31.030 | 1.00 | 34.24 | 6 |
| | ATOM | 1052 | CG | LEU | B | 400 | -21.470 | 79.642 | 29.726 | 1.00 | 35.10 | 6 |
| | ATOM | 1053 | CD1 | LEU | B | 400 | -20.121 | 80.304 | 29.917 | 1.00 | 26.60 | 6 |
| 40 | ATOM | 1054 | CD2 | LEU | B | 400 | -21.326 | 78.488 | 28.759 | 1.00 | 29.44 | 6 |
| | ATOM | 1055 | C | LEU | B | 400 | -23.430 | 77.376 | 32.145 | 1.00 | 38.84 | 6 |
| | ATOM | 1056 | O | LEU | B | 400 | -23.366 | 76.157 | 32.007 | 1.00 | 40.38 | 8 |
| | ATOM | 1057 | N | LEU | B | 401 | -23.639 | 77.968 | 33.321 | 1.00 | 42.79 | 7 |
| | ATOM | 1058 | CA | LEU | B | 401 | -23.801 | 77.181 | 34.537 | 1.00 | 43.48 | 6 |
| 45 | ATOM | 1059 | CB | LEU | B | 401 | -24.226 | 78.067 | 35.712 | 1.00 | 44.73 | 6 |
| | ATOM | 1060 | CG | LEU | B | 401 | -24.378 | 77.303 | 37.012 | 1.00 | 51.39 | 6 |
| | ATOM | 1061 | CD1 | LEU | B | 401 | -22.990 | 76.844 | 37.484 | 1.00 | 50.11 | 6 |
| | ATOM | 1062 | CD2 | LEU | B | 401 | -25.027 | 78.163 | 38.083 | 1.00 | 49.30 | 6 |
| | ATOM | 1063 | C | LEU | B | 401 | -24.854 | 76.095 | 34.311 | 1.00 | 41.62 | 6 |
| 50 | ATOM | 1064 | O | LEU | B | 401 | -24.576 | 74.900 | 34.427 | 1.00 | 45.14 | 8 |
| | ATOM | 1065 | N | ALA | B | 402 | -26.068 | 76.532 | 33.997 | 1.00 | 37.92 | 7 |
| | ATOM | 1066 | CA | ALA | B | 402 | -27.177 | 75.631 | 33.752 | 1.00 | 29.90 | 6 |
| | ATOM | 1067 | CB | ALA | B | 402 | -28.361 | 76.433 | 33.200 | 1.00 | 30.70 | 6 |
| | ATOM | 1068 | C | ALA | B | 402 | -26.779 | 74.521 | 32.773 | 1.00 | 28.88 | 6 |
| 55 | ATOM | 1069 | O | ALA | B | 402 | -27.078 | 73.347 | 32.996 | 1.00 | 32.14 | 8 |
| | ATOM | 1070 | N | PHE | B | 403 | -26.091 | 74.908 | 31.698 | 1.00 | 31.07 | 7 |
| | ATOM | 1071 | CA | PHE | B | 403 | -25.655 | 73.970 | 30.673 | 1.00 | 29.90 | 6 |
| | ATOM | 1072 | CB | PHE | B | 403 | -24.847 | 74.715 | 29.607 | 1.00 | 27.03 | 6 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 1073 | CG | PHE | B | 403 | -24.557 | 73.908 | 28.359 | 1.00 | 26.97 | 6 |
| | ATOM | 1074 | CD1 | PHE | B | 403 | -23.916 | 74.494 | 27.272 | 1.00 | 25.55 | 6 |
| | ATOM | 1075 | CD2 | PHE | B | 403 | -24.939 | 72.583 | 28.271 | 1.00 | 19.75 | 6 |
| | ATOM | 1076 | CE1 | PHE | B | 403 | -23.670 | 73.765 | 26.104 | 1.00 | 27.90 | 6 |
| | ATOM | 1077 | CE2 | PHE | B | 403 | -24.693 | 71.848 | 27.102 | 1.00 | 22.56 | 6 |
| 10 | ATOM | 1078 | CZ | PHE | B | 403 | -24.057 | 72.439 | 26.020 | 1.00 | 22.24 | 6 |
| | ATOM | 1079 | C | PHE | B | 403 | -24.810 | 72.902 | 31.329 | 1.00 | 28.82 | 6 |
| | ATOM | 1080 | O | PHE | B | 403 | -25.092 | 71.726 | 31.205 | 1.00 | 26.00 | 8 |
| | ATOM | 1081 | N | GLU | B | 404 | -23.776 | 73.335 | 32.037 | 1.00 | 30.25 | 7 |
| | ATOM | 1082 | CA | GLU | B | 404 | -22.865 | 72.419 | 32.712 | 1.00 | 34.03 | 6 |
| 15 | ATOM | 1083 | CB | GLU | B | 404 | -21.835 | 73.215 | 33.527 | 1.00 | 39.45 | 6 |
| | ATOM | 1084 | CG | GLU | B | 404 | -20.654 | 72.384 | 34.068 | 1.00 | 47.68 | 6 |
| | ATOM | 1085 | CD | GLU | B | 404 | -19.750 | 73.129 | 34.996 | 1.00 | 54.02 | 6 |
| | ATOM | 1086 | OE1 | GLU | B | 404 | -19.372 | 74.290 | 34.701 | 1.00 | 57.27 | 8 |
| | ATOM | 1087 | OE2 | GLU | B | 404 | -19.369 | 72.555 | 36.048 | 1.00 | 63.85 | 8 |
| 20 | ATOM | 1088 | C | GLU | B | 404 | -23.645 | 71.509 | 33.642 | 1.00 | 36.01 | 6 |
| | ATOM | 1089 | O | GLU | B | 404 | -23.470 | 70.292 | 33.640 | 1.00 | 38.64 | 8 |
| | ATOM | 1090 | N | HIS | B | 405 | -24.492 | 72.131 | 34.458 | 1.00 | 29.56 | 7 |
| | ATOM | 1091 | CA | HIS | B | 405 | -25.306 | 71.387 | 35.405 | 1.00 | 31.69 | 6 |
| | ATOM | 1092 | CB | HIS | B | 405 | -26.245 | 72.324 | 36.173 | 1.00 | 33.75 | 6 |
| 25 | ATOM | 1093 | CG | HIS | B | 405 | -25.536 | 73.185 | 37.163 | 1.00 | 34.75 | 6 |
| | ATOM | 1094 | CD2 | HIS | B | 405 | -24.234 | 73.286 | 37.524 | 1.00 | 34.58 | 6 |
| | ATOM | 1095 | ND1 | HIS | B | 405 | -26.223 | 74.101 | 37.969 | 1.00 | 32.43 | 7 |
| | ATOM | 1096 | CE1 | HIS | B | 405 | -25.334 | 74.703 | 38.769 | 1.00 | 36.15 | 6 |
| | ATOM | 1097 | NE2 | HIS | B | 405 | -24.139 | 74.222 | 38.511 | 1.00 | 39.84 | 7 |
| 30 | ATOM | 1098 | C | HIS | B | 405 | -26.106 | 70.342 | 34.648 | 1.00 | 34.21 | 6 |
| | ATOM | 1099 | O | HIS | B | 405 | -26.087 | 69.160 | 35.006 | 1.00 | 37.06 | 8 |
| | ATOM | 1100 | N | TYR | B | 406 | -26.806 | 70.776 | 33.598 | 1.00 | 30.83 | 7 |
| | ATOM | 1101 | CA | TYR | B | 406 | -27.592 | 69.853 | 32.796 | 1.00 | 28.85 | 6 |
| | ATOM | 1102 | CB | TYR | B | 406 | -28.192 | 70.537 | 31.579 | 1.00 | 31.48 | 6 |
| 35 | ATOM | 1103 | CG | TYR | B | 406 | -28.991 | 69.576 | 30.730 | 1.00 | 23.49 | 6 |
| | ATOM | 1104 | CD1 | TYR | B | 406 | -30.179 | 69.047 | 31.196 | 1.00 | 19.42 | 6 |
| | ATOM | 1105 | CE1 | TYR | B | 406 | -30.893 | 68.128 | 30.441 | 1.00 | 23.80 | 6 |
| | ATOM | 1106 | CD2 | TYR | B | 406 | -28.525 | 69.152 | 29.496 | 1.00 | 21.81 | 6 |
| | ATOM | 1107 | CE2 | TYR | B | 406 | -29.241 | 68.228 | 28.740 | 1.00 | 24.64 | 6 |
| 40 | ATOM | 1108 | CZ | TYR | B | 406 | -30.420 | 67.713 | 29.217 | 1.00 | 21.56 | 6 |
| | ATOM | 1109 | OH | TYR | B | 406 | -31.120 | 66.802 | 28.480 | 1.00 | 24.96 | 8 |
| | ATOM | 1110 | C | TYR | B | 406 | -26.697 | 68.725 | 32.304 | 1.00 | 24.24 | 6 |
| | ATOM | 1111 | O | TYR | B | 406 | -27.155 | 67.609 | 32.110 | 1.00 | 27.08 | 8 |
| | ATOM | 1112 | N | ILE | B | 407 | -25.422 | 69.056 | 32.084 | 1.00 | 25.76 | 7 |
| 45 | ATOM | 1113 | CA | ILE | B | 407 | -24.428 | 68.092 | 31.628 | 1.00 | 33.75 | 6 |
| | ATOM | 1114 | CB | ILE | B | 407 | -23.090 | 68.778 | 31.274 | 1.00 | 34.23 | 6 |
| | ATOM | 1115 | CG2 | ILE | B | 407 | -21.959 | 67.774 | 31.230 | 1.00 | 32.46 | 6 |
| | ATOM | 1116 | CG1 | ILE | B | 407 | -23.214 | 69.514 | 29.936 | 1.00 | 43.30 | 6 |
| | ATOM | 1117 | CD1 | ILE | B | 407 | -23.655 | 68.612 | 28.804 | 1.00 | 40.40 | 6 |
| 50 | ATOM | 1118 | C | ILE | B | 407 | -24.191 | 67.004 | 32.658 | 1.00 | 39.03 | 6 |
| | ATOM | 1119 | O | ILE | B | 407 | -24.178 | 65.806 | 32.343 | 1.00 | 35.18 | 8 |
| | ATOM | 1120 | N | ASN | B | 408 | -23.990 | 67.425 | 33.894 | 1.00 | 37.25 | 7 |
| | ATOM | 1121 | CA | ASN | B | 408 | -23.739 | 66.475 | 34.943 | 1.00 | 37.01 | 6 |
| | ATOM | 1122 | CB | ASN | B | 408 | -23.524 | 67.221 | 36.256 | 1.00 | 32.27 | 6 |
| 55 | ATOM | 1123 | CG | ASN | B | 408 | -22.296 | 68.137 | 36.202 | 1.00 | 33.56 | 6 |
| | ATOM | 1124 | OD1 | ASN | B | 408 | -21.194 | 67.696 | 35.823 | 1.00 | 31.99 | 8 |
| | ATOM | 1125 | ND2 | ASN | B | 408 | -22.478 | 69.397 | 36.604 | 1.00 | 31.23 | 7 |
| | ATOM | 1126 | C | ASN | B | 408 | -24.876 | 65.453 | 35.036 | 1.00 | 38.14 | 6 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 1127 | O | ASN | B | 408 | -24.624 | 64.253 | 35.105 | 1.00 | 42.16 | 8 |
| | ATOM | 1128 | N | TYR | B | 409 | -26.122 | 65.924 | 35.003 | 1.00 | 35.62 | 7 |
| | ATOM | 1129 | CA | TYR | B | 409 | -27.273 | 65.024 | 35.073 | 1.00 | 35.91 | 6 |
| | ATOM | 1130 | CB | TYR | B | 409 | -28.597 | 65.787 | 34.931 | 1.00 | 34.41 | 6 |
| | ATOM | 1131 | CG | TYR | B | 409 | -29.788 | 64.868 | 34.685 | 1.00 | 38.73 | 6 |
| 10 | ATOM | 1132 | CD1 | TYR | B | 409 | -30.064 | 63.819 | 35.549 | 1.00 | 41.34 | 6 |
| | ATOM | 1133 | CE1 | TYR | B | 409 | -31.130 | 62.962 | 35.309 | 1.00 | 47.16 | 6 |
| | ATOM | 1134 | CD2 | TYR | B | 409 | -30.613 | 65.037 | 33.579 | 1.00 | 46.20 | 6 |
| | ATOM | 1135 | CE2 | TYR | B | 409 | -31.684 | 64.176 | 33.341 | 1.00 | 50.74 | 6 |
| | ATOM | 1136 | CZ | TYR | B | 409 | -31.942 | 63.143 | 34.206 | 1.00 | 50.88 | 6 |
| 15 | ATOM | 1137 | OH | TYR | B | 409 | -33.002 | 62.312 | 33.978 | 1.00 | 53.14 | 8 |
| | ATOM | 1138 | C | TYR | B | 409 | -27.215 | 64.020 | 33.951 | 1.00 | 38.16 | 6 |
| | ATOM | 1139 | O | TYR | B | 409 | -27.558 | 62.857 | 34.111 | 1.00 | 41.83 | 8 |
| | ATOM | 1140 | N | ARG | B | 410 | -26.824 | 64.528 | 32.796 | 1.00 | 42.25 | 7 |
| | ATOM | 1141 | CA | ARG | B | 410 | -26.734 | 63.739 | 31.594 | 1.00 | 42.83 | 6 |
| 20 | ATOM | 1142 | CB | ARG | B | 410 | -26.350 | 64.646 | 30.441 | 1.00 | 36.83 | 6 |
| | ATOM | 1143 | CG | ARG | B | 410 | -27.440 | 65.585 | 29.945 | 1.00 | 34.32 | 6 |
| | ATOM | 1144 | CD | ARG | B | 410 | -28.284 | 64.863 | 28.917 | 1.00 | 36.62 | 6 |
| | ATOM | 1145 | NE | ARG | B | 410 | -27.455 | 64.378 | 27.829 | 1.00 | 38.64 | 7 |
| | ATOM | 1146 | CZ | ARG | B | 410 | -27.926 | 63.656 | 26.824 | 1.00 | 35.73 | 6 |
| 25 | ATOM | 1147 | NH1 | ARG | B | 410 | -29.234 | 63.379 | 26.782 | 1.00 | 33.17 | 7 |
| | ATOM | 1148 | NH2 | ARG | B | 410 | -27.095 | 63.227 | 25.868 | 1.00 | 32.70 | 7 |
| | ATOM | 1149 | C | ARG | B | 410 | -25.688 | 62.664 | 31.733 | 1.00 | 46.67 | 6 |
| | ATOM | 1150 | O | ARG | B | 410 | -25.859 | 61.547 | 31.257 | 1.00 | 41.78 | 8 |
| | ATOM | 1151 | N | LYS | B | 411 | -24.602 | 63.028 | 32.413 | 1.00 | 52.99 | 7 |
| 30 | ATOM | 1152 | CA | LYS | B | 411 | -23.471 | 62.145 | 32.609 | 1.00 | 58.32 | 6 |
| | ATOM | 1153 | CB | LYS | B | 411 | -23.684 | 61.249 | 33.833 | 1.00 | 64.99 | 6 |
| | ATOM | 1154 | CG | LYS | B | 411 | -24.998 | 60.544 | 33.968 | 1.00 | 70.48 | 6 |
| | ATOM | 1155 | CD | LYS | B | 411 | -25.070 | 59.887 | 35.349 | 1.00 | 77.18 | 6 |
| | ATOM | 1156 | CE | LYS | B | 411 | -26.272 | 58.944 | 35.474 | 1.00 | 84.30 | 6 |
| 35 | ATOM | 1157 | NZ | LYS | B | 411 | -26.286 | 58.242 | 36.809 | 1.00 | 86.48 | 7 |
| | ATOM | 1158 | C | LYS | B | 411 | -23.172 | 61.341 | 31.365 | 1.00 | 56.66 | 6 |
| | ATOM | 1159 | O | LYS | B | 411 | -23.574 | 60.199 | 31.210 | 1.00 | 55.47 | 8 |
| | ATOM | 1160 | N | HIS | B | 412 | -22.458 | 62.026 | 30.479 | 1.00 | 54.67 | 7 |
| | ATOM | 1161 | CA | HIS | B | 412 | -22.019 | 61.474 | 29.214 | 1.00 | 48.67 | 6 |
| 40 | ATOM | 1162 | CB | HIS | B | 412 | -21.500 | 62.599 | 28.310 | 1.00 | 43.14 | 6 |
| | ATOM | 1163 | CG | HIS | B | 412 | -22.559 | 63.501 | 27.784 | 1.00 | 41.36 | 6 |
| | ATOM | 1164 | CD2 | HIS | B | 412 | -23.159 | 64.603 | 28.299 | 1.00 | 35.44 | 6 |
| | ATOM | 1165 | ND1 | HIS | B | 412 | -23.163 | 63.290 | 26.539 | 1.00 | 38.19 | 7 |
| | ATOM | 1166 | CE1 | HIS | B | 412 | -24.076 | 64.238 | 26.353 | 1.00 | 34.75 | 6 |
| 45 | ATOM | 1167 | NE2 | HIS | B | 412 | -24.090 | 65.034 | 27.396 | 1.00 | 35.52 | 7 |
| | ATOM | 1168 | C | HIS | B | 412 | -20.894 | 60.596 | 29.644 | 1.00 | 46.35 | 6 |
| | ATOM | 1169 | O | HIS | B | 412 | -20.218 | 60.892 | 30.644 | 1.00 | 42.73 | 8 |
| | ATOM | 1170 | N | HIS | B | 413 | -20.708 | 59.469 | 28.973 | 1.00 | 48.92 | 7 |
| | ATOM | 1171 | CA | HIS | B | 413 | -19.593 | 58.614 | 29.371 | 1.00 | 53.15 | 6 |
| 50 | ATOM | 1172 | CB | HIS | B | 413 | -20.022 | 57.147 | 29.421 | 1.00 | 55.27 | 6 |
| | ATOM | 1173 | CG | HIS | B | 413 | -20.814 | 56.823 | 30.636 | 1.00 | 58.77 | 6 |
| | ATOM | 1174 | CD2 | HIS | B | 413 | -22.019 | 56.223 | 30.822 | 1.00 | 61.65 | 6 |
| | ATOM | 1175 | ND1 | HIS | B | 413 | -20.360 | 57.159 | 31.921 | 1.00 | 60.31 | 7 |
| | ATOM | 1176 | CE1 | HIS | B | 413 | -21.267 | 56.758 | 32.809 | 1.00 | 63.01 | 6 |
| 55 | ATOM | 1177 | NE2 | HIS | B | 413 | -22.270 | 56.193 | 32.171 | 1.00 | 62.93 | 7 |
| | ATOM | 1178 | C | HIS | B | 413 | -18.426 | 58.862 | 28.438 | 1.00 | 53.19 | 6 |
| | ATOM | 1179 | O | HIS | B | 413 | -17.975 | 57.996 | 27.699 | 1.00 | 54.93 | 8 |
| | ATOM | 1180 | N | VAL | B | 414 | -17.970 | 60.113 | 28.521 | 1.00 | 53.77 | 7 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 1181 | CA | VAL | B | 414 | -16.845 | 60.674 | 27.788 | 1.00 | 51.06 | 6 |
| | ATOM | 1182 | CB | VAL | B | 414 | -17.317 | 61.498 | 26.586 | 1.00 | 51.49 | 6 |
| | ATOM | 1183 | CG1 | VAL | B | 414 | -16.133 | 62.122 | 25.891 | 1.00 | 45.22 | 6 |
| | ATOM | 1184 | CG2 | VAL | B | 414 | -18.095 | 60.631 | 25.617 | 1.00 | 52.67 | 6 |
| | ATOM | 1185 | C | VAL | B | 414 | -16.096 | 61.557 | 28.775 | 1.00 | 54.28 | 6 |
| 10 | ATOM | 1186 | O | VAL | B | 414 | -16.700 | 62.283 | 29.574 | 1.00 | 55.49 | 8 |
| | ATOM | 1187 | N | THR | B | 415 | -14.770 | 61.466 | 28.742 | 1.00 | 56.28 | 7 |
| | ATOM | 1188 | CA | THR | B | 415 | -13.919 | 62.234 | 29.669 | 1.00 | 57.83 | 6 |
| | ATOM | 1189 | CB | THR | B | 415 | -12.488 | 61.686 | 29.658 | 1.00 | 59.64 | 6 |
| | ATOM | 1190 | OG1 | THR | B | 415 | -11.618 | 62.572 | 30.373 | 1.00 | 66.69 | 8 |
| 15 | ATOM | 1191 | CG2 | THR | B | 415 | -11.988 | 61.483 | 28.227 | 1.00 | 59.42 | 6 |
| | ATOM | 1192 | C | THR | B | 415 | -13.840 | 63.726 | 29.352 | 1.00 | 56.98 | 6 |
| | ATOM | 1193 | O | THR | B | 415 | -13.987 | 64.135 | 28.216 | 1.00 | 55.70 | 8 |
| | ATOM | 1194 | N | HIS | B | 416 | -13.598 | 64.522 | 30.387 | 1.00 | 57.44 | 7 |
| | ATOM | 1195 | CA | HIS | B | 416 | -13.485 | 65.972 | 30.237 | 1.00 | 57.34 | 6 |
| 20 | ATOM | 1196 | CB | HIS | B | 416 | -12.114 | 66.326 | 29.653 | 1.00 | 61.35 | 6 |
| | ATOM | 1197 | CG | HIS | B | 416 | -10.968 | 65.931 | 30.513 | 1.00 | 69.78 | 6 |
| | ATOM | 1198 | CD2 | HIS | B | 416 | -9.930 | 65.082 | 30.307 | 1.00 | 71.42 | 6 |
| | ATOM | 1199 | ND1 | HIS | B | 416 | -10.756 | 66.480 | 31.787 | 1.00 | 72.49 | 7 |
| | ATOM | 1200 | CE1 | HIS | B | 416 | -9.631 | 65.973 | 32.281 | 1.00 | 75.50 | 6 |
| 25 | ATOM | 1201 | NE2 | HIS | B | 416 | -9.120 | 65.131 | 31.408 | 1.00 | 73.91 | 7 |
| | ATOM | 1202 | C | HIS | B | 416 | -14.560 | 66.515 | 29.320 | 1.00 | 53.79 | 6 |
| | ATOM | 1203 | O | HIS | B | 416 | -14.334 | 67.477 | 28.591 | 1.00 | 52.81 | 8 |
| | ATOM | 1204 | N | PHE | B | 417 | -15.746 | 65.921 | 29.372 | 1.00 | 48.05 | 7 |
| | ATOM | 1205 | CA | PHE | B | 417 | -16.841 | 66.329 | 28.505 | 1.00 | 47.99 | 6 |
| 30 | ATOM | 1206 | CB | PHE | B | 417 | -18.152 | 65.694 | 28.937 | 1.00 | 46.11 | 6 |
| | ATOM | 1207 | CG | PHE | B | 417 | -19.233 | 65.781 | 27.898 | 1.00 | 44.27 | 6 |
| | ATOM | 1208 | CD1 | PHE | B | 417 | -19.280 | 64.856 | 26.870 | 1.00 | 41.79 | 6 |
| | ATOM | 1209 | CD2 | PHE | B | 417 | -20.118 | 66.846 | 27.893 | 1.00 | 40.23 | 6 |
| | ATOM | 1210 | CE1 | PHE | B | 417 | -20.233 | 64.959 | 25.869 | 1.00 | 44.30 | 6 |
| 35 | ATOM | 1211 | CE2 | PHE | B | 417 | -21.072 | 66.955 | 26.893 | 1.00 | 36.80 | 6 |
| | ATOM | 1212 | CZ | PHE | B | 417 | -21.119 | 66.016 | 25.866 | 1.00 | 40.69 | 6 |
| | ATOM | 1213 | C | PHE | B | 417 | -17.020 | 67.833 | 28.423 | 1.00 | 46.69 | 6 |
| | ATOM | 1214 | O | PHE | B | 417 | -16.799 | 68.423 | 27.380 | 1.00 | 43.35 | 8 |
| | ATOM | 1215 | N | TRP | B | 418 | -17.448 | 68.452 | 29.516 | 1.00 | 45.14 | 7 |
| 40 | ATOM | 1216 | CA | TRP | B | 418 | -17.681 | 69.889 | 29.508 | 1.00 | 44.89 | 6 |
| | ATOM | 1217 | CB | TRP | B | 418 | -18.045 | 70.398 | 30.898 | 1.00 | 42.24 | 6 |
| | ATOM | 1218 | CG | TRP | B | 418 | -18.162 | 71.905 | 31.018 | 1.00 | 47.11 | 6 |
| | ATOM | 1219 | CD2 | TRP | B | 418 | -19.298 | 72.699 | 30.620 | 1.00 | 46.98 | 6 |
| | ATOM | 1220 | CE2 | TRP | B | 418 | -18.953 | 74.061 | 30.850 | 1.00 | 48.94 | 6 |
| 45 | ATOM | 1221 | CE3 | TRP | B | 418 | -20.560 | 72.401 | 30.086 | 1.00 | 45.23 | 6 |
| | ATOM | 1222 | CD1 | TRP | B | 418 | -17.223 | 72.778 | 31.462 | 1.00 | 46.24 | 6 |
| | ATOM | 1223 | NE1 | TRP | B | 418 | -17.690 | 74.071 | 31.368 | 1.00 | 50.63 | 7 |
| | ATOM | 1224 | CZ2 | TRP | B | 418 | -19.819 | 75.109 | 30.571 | 1.00 | 45.46 | 6 |
| | ATOM | 1225 | CZ3 | TRP | B | 418 | -21.422 | 73.447 | 29.809 | 1.00 | 44.50 | 6 |
| 50 | ATOM | 1226 | CH2 | TRP | B | 418 | -21.065 | 74.777 | 30.039 | 1.00 | 47.55 | 6 |
| | ATOM | 1227 | C | TRP | B | 418 | -16.502 | 70.662 | 28.956 | 1.00 | 43.88 | 6 |
| | ATOM | 1228 | O | TRP | B | 418 | -16.671 | 71.424 | 27.986 | 1.00 | 43.17 | 8 |
| | ATOM | 1229 | N | PRO | B | 419 | -15.292 | 70.490 | 29.519 | 1.00 | 43.55 | 7 |
| | ATOM | 1230 | CD | PRO | B | 419 | -14.967 | 69.551 | 30.599 | 1.00 | 41.52 | 6 |
| 55 | ATOM | 1231 | CA | PRO | B | 419 | -14.120 | 71.223 | 29.011 | 1.00 | 41.48 | 6 |
| | ATOM | 1232 | CB | PRO | B | 419 | -12.956 | 70.582 | 29.724 | 1.00 | 39.21 | 6 |
| | ATOM | 1233 | CG | PRO | B | 419 | -13.521 | 69.703 | 30.774 | 1.00 | 39.25 | 6 |
| | ATOM | 1234 | C | PRO | B | 419 | -14.035 | 71.067 | 27.479 | 1.00 | 36.28 | 6 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 1235 | O | PRO | B | 419 | -13.690 | 72.001 | 26.754 | 1.00 | 37.08 | 8 |
| | ATOM | 1236 | N | LYS | B | 420 | -14.330 | 69.871 | 26.976 | 1.00 | 35.96 | 7 |
| | ATOM | 1237 | CA | LYS | B | 420 | -14.278 | 69.609 | 25.538 | 1.00 | 40.82 | 6 |
| | ATOM | 1238 | CB | LYS | B | 420 | -14.452 | 68.103 | 25.271 | 1.00 | 40.78 | 6 |
| | ATOM | 1239 | CG | LYS | B | 420 | -13.349 | 67.214 | 25.830 | 1.00 | 48.62 | 6 |
| 10 | ATOM | 1240 | CD | LYS | B | 420 | -13.565 | 65.746 | 25.480 | 1.00 | 55.12 | 6 |
| | ATOM | 1241 | CE | LYS | B | 420 | -12.427 | 64.892 | 26.017 | 1.00 | 53.26 | 6 |
| | ATOM | 1242 | NZ | LYS | B | 420 | -12.582 | 63.457 | 25.608 | 1.00 | 52.69 | 7 |
| | ATOM | 1243 | C | LYS | B | 420 | -15.414 | 70.374 | 24.875 | 1.00 | 40.29 | 6 |
| | ATOM | 1244 | O | LYS | B | 420 | -15.225 | 71.015 | 23.851 | 1.00 | 39.66 | 8 |
| 15 | ATOM | 1245 | N | LEU | B | 421 | -16.591 | 70.300 | 25.499 | 1.00 | 38.33 | 7 |
| | ATOM | 1246 | CA | LEU | B | 421 | -17.796 | 70.958 | 25.001 | 1.00 | 37.60 | 6 |
| | ATOM | 1247 | CB | LEU | B | 421 | -18.970 | 70.702 | 25.965 | 1.00 | 43.66 | 6 |
| | ATOM | 1248 | CG | LEU | B | 421 | -20.370 | 70.850 | 25.418 | 1.00 | 46.50 | 6 |
| | ATOM | 1249 | CD1 | LEU | B | 421 | -20.529 | 69.890 | 24.255 | 1.00 | 45.15 | 6 |
| 20 | ATOM | 1250 | CD2 | LEU | B | 421 | -21.383 | 70.538 | 26.486 | 1.00 | 51.31 | 6 |
| | ATOM | 1251 | C | LEU | B | 421 | -17.547 | 72.452 | 24.823 | 1.00 | 39.59 | 6 |
| | ATOM | 1252 | O | LEU | B | 421 | -17.975 | 73.035 | 23.836 | 1.00 | 40.66 | 8 |
| | ATOM | 1253 | N | LEU | B | 422 | -16.847 | 73.059 | 25.780 | 1.00 | 39.57 | 7 |
| | ATOM | 1254 | CA | LEU | B | 422 | -16.534 | 74.478 | 25.715 | 1.00 | 38.63 | 6 |
| 25 | ATOM | 1255 | CB | LEU | B | 422 | -15.829 | 74.936 | 26.992 | 1.00 | 41.79 | 6 |
| | ATOM | 1256 | CG | LEU | B | 422 | -16.714 | 75.149 | 28.191 | 1.00 | 42.74 | 6 |
| | ATOM | 1257 | CD1 | LEU | B | 422 | -15.911 | 75.685 | 29.360 | 1.00 | 42.89 | 6 |
| | ATOM | 1258 | CD2 | LEU | B | 422 | -17.783 | 76.162 | 27.813 | 1.00 | 39.27 | 6 |
| | ATOM | 1259 | C | LEU | B | 422 | -15.677 | 74.788 | 24.513 | 1.00 | 40.47 | 6 |
| 30 | ATOM | 1260 | O | LEU | B | 422 | -15.823 | 75.846 | 23.917 | 1.00 | 47.83 | 8 |
| | ATOM | 1261 | N | MET | B | 423 | -14.789 | 73.853 | 24.168 | 1.00 | 34.27 | 7 |
| | ATOM | 1262 | CA | MET | B | 423 | -13.907 | 74.019 | 23.024 | 1.00 | 35.25 | 6 |
| | ATOM | 1263 | CB | MET | B | 423 | -12.920 | 72.858 | 22.922 | 1.00 | 32.56 | 6 |
| | ATOM | 1264 | CG | MET | B | 423 | -12.013 | 72.703 | 24.125 | 1.00 | 40.70 | 6 |
| 35 | ATOM | 1265 | SD | MET | B | 423 | -10.345 | 72.007 | 23.784 | 1.00 | 47.65 | 16 |
| | ATOM | 1266 | CE | MET | B | 423 | -10.770 | 70.538 | 22.761 | 1.00 | 47.16 | 6 |
| | ATOM | 1267 | C | MET | B | 423 | -14.709 | 74.100 | 21.738 | 1.00 | 35.13 | 6 |
| | ATOM | 1268 | O | MET | B | 423 | -14.341 | 74.807 | 20.803 | 1.00 | 29.85 | 8 |
| | ATOM | 1269 | N | LYS | B | 424 | -15.811 | 73.361 | 21.704 | 1.00 | 31.56 | 7 |
| 40 | ATOM | 1270 | CA | LYS | B | 424 | -16.676 | 73.354 | 20.544 | 1.00 | 32.29 | 6 |
| | ATOM | 1271 | CB | LYS | B | 424 | -17.783 | 72.316 | 20.736 | 1.00 | 30.56 | 6 |
| | ATOM | 1272 | CG | LYS | B | 424 | -17.257 | 70.879 | 20.843 | 1.00 | 30.07 | 6 |
| | ATOM | 1273 | CD | LYS | B | 424 | -16.444 | 70.510 | 19.611 | 1.00 | 33.22 | 6 |
| | ATOM | 1274 | CE | LYS | B | 424 | -15.795 | 69.136 | 19.706 | 1.00 | 28.75 | 6 |
| 45 | ATOM | 1275 | NZ | LYS | B | 424 | -14.655 | 69.067 | 20.678 | 1.00 | 31.01 | 7 |
| | ATOM | 1276 | C | LYS | B | 424 | -17.248 | 74.754 | 20.304 | 1.00 | 29.26 | 6 |
| | ATOM | 1277 | O | LYS | B | 424 | -17.439 | 75.149 | 19.166 | 1.00 | 30.22 | 8 |
| | ATOM | 1278 | N | VAL | B | 425 | -17.495 | 75.499 | 21.385 | 1.00 | 23.53 | 7 |
| | ATOM | 1279 | CA | VAL | B | 425 | -18.014 | 76.852 | 21.278 | 1.00 | 28.91 | 6 |
| 50 | ATOM | 1280 | CB | VAL | B | 425 | -18.278 | 77.458 | 22.663 | 1.00 | 29.44 | 6 |
| | ATOM | 1281 | CG1 | VAL | B | 425 | -18.633 | 78.915 | 22.547 | 1.00 | 28.81 | 6 |
| | ATOM | 1282 | CG2 | VAL | B | 425 | -19.401 | 76.733 | 23.354 | 1.00 | 31.22 | 6 |
| | ATOM | 1283 | C | VAL | B | 425 | -17.001 | 77.682 | 20.498 | 1.00 | 32.03 | 6 |
| | ATOM | 1284 | O | VAL | B | 425 | -17.368 | 78.465 | 19.629 | 1.00 | 31.95 | 8 |
| 55 | ATOM | 1285 | N | THR | B | 426 | -15.721 | 77.508 | 20.827 | 1.00 | 33.61 | 7 |
| | ATOM | 1286 | CA | THR | B | 426 | -14.645 | 78.221 | 20.137 | 1.00 | 30.76 | 6 |
| | ATOM | 1287 | CB | THR | B | 426 | -13.270 | 77.912 | 20.761 | 1.00 | 32.34 | 6 |
| | ATOM | 1288 | OG1 | THR | B | 426 | -13.073 | 78.697 | 21.941 | 1.00 | 33.07 | 8 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 1289 | CG2 | THR | B | 426 | -12.153 | 78.174 | 19.782 | 1.00 | 25.40 | 6 |
| | ATOM | 1290 | C | THR | B | 426 | -14.677 | 77.742 | 18.706 | 1.00 | 32.53 | 6 |
| | ATOM | 1291 | O | THR | B | 426 | -14.639 | 78.530 | 17.763 | 1.00 | 35.19 | 8 |
| | ATOM | 1292 | N | ASP | B | 427 | -14.749 | 76.425 | 18.566 | 1.00 | 28.83 | 7 |
| | ATOM | 1293 | CA | ASP | B | 427 | -14.796 | 75.807 | 17.257 | 1.00 | 35.12 | 6 |
| 10 | ATOM | 1294 | CB | ASP | B | 427 | -15.096 | 74.302 | 17.380 | 1.00 | 39.14 | 6 |
| | ATOM | 1295 | CG | ASP | B | 427 | -13.910 | 73.496 | 17.806 | 1.00 | 45.80 | 6 |
| | ATOM | 1296 | OD1 | ASP | B | 427 | -12.786 | 73.774 | 17.348 | 1.00 | 41.97 | 8 |
| | ATOM | 1297 | OD2 | ASP | B | 427 | -14.064 | 72.517 | 18.583 | 1.00 | 50.06 | 8 |
| | ATOM | 1298 | C | ASP | B | 427 | -15.883 | 76.502 | 16.429 | 1.00 | 33.94 | 6 |
| 15 | ATOM | 1299 | O | ASP | B | 427 | -15.673 | 76.815 | 15.262 | 1.00 | 38.02 | 8 |
| | ATOM | 1300 | N | LEU | B | 428 | -17.040 | 76.741 | 17.048 | 1.00 | 27.15 | 7 |
| | ATOM | 1301 | CA | LEU | B | 428 | -18.154 | 77.388 | 16.367 | 1.00 | 29.99 | 6 |
| | ATOM | 1302 | CB | LEU | B | 428 | -19.448 | 77.190 | 17.168 | 1.00 | 22.49 | 6 |
| | ATOM | 1303 | CG | LEU | B | 428 | -20.086 | 75.818 | 17.089 | 1.00 | 25.54 | 6 |
| 20 | ATOM | 1304 | CD1 | LEU | B | 428 | -21.282 | 75.729 | 18.012 | 1.00 | 20.60 | 6 |
| | ATOM | 1305 | CD2 | LEU | B | 428 | -20.509 | 75.564 | 15.651 | 1.00 | 17.24 | 6 |
| | ATOM | 1306 | C | LEU | B | 428 | -17.901 | 78.863 | 16.103 | 1.00 | 28.94 | 6 |
| | ATOM | 1307 | O | LEU | B | 428 | -18.328 | 79.388 | 15.076 | 1.00 | 31.26 | 8 |
| | ATOM | 1308 | N | ARG | B | 429 | -17.213 | 79.524 | 17.035 | 1.00 | 27.64 | 7 |
| 25 | ATOM | 1309 | CA | ARG | B | 429 | -16.894 | 80.937 | 16.883 | 1.00 | 28.13 | 6 |
| | ATOM | 1310 | CB | ARG | B | 429 | -16.274 | 81.507 | 18.160 | 1.00 | 29.59 | 6 |
| | ATOM | 1311 | CG | ARG | B | 429 | -17.246 | 81.752 | 19.302 | 1.00 | 34.85 | 6 |
| | ATOM | 1312 | CD | ARG | B | 429 | -16.626 | 82.653 | 20.372 | 1.00 | 47.18 | 6 |
| | ATOM | 1313 | NE | ARG | B | 429 | -17.373 | 82.714 | 21.620 | 1.00 | 57.93 | 7 |
| 30 | ATOM | 1314 | CZ | ARG | B | 429 | -18.632 | 83.124 | 21.716 | 1.00 | 63.62 | 6 |
| | ATOM | 1315 | NH1 | ARG | B | 429 | -19.263 | 83.579 | 20.622 | 1.00 | 60.71 | 7 |
| | ATOM | 1316 | NH2 | ARG | B | 429 | -19.238 | 83.130 | 22.916 | 1.00 | 62.38 | 7 |
| | ATOM | 1317 | C | ARG | B | 429 | -15.930 | 81.146 | 15.728 | 1.00 | 29.81 | 6 |
| | ATOM | 1318 | O | ARG | B | 429 | -16.101 | 82.061 | 14.933 | 1.00 | 30.81 | 8 |
| 35 | ATOM | 1319 | N | MET | B | 430 | -14.908 | 80.295 | 15.670 | 1.00 | 29.64 | 7 |
| | ATOM | 1320 | CA | MET | B | 430 | -13.920 | 80.343 | 14.614 | 1.00 | 34.72 | 6 |
| | ATOM | 1321 | CB | MET | B | 430 | -12.939 | 79.192 | 14.763 | 1.00 | 34.97 | 6 |
| | ATOM | 1322 | CG | MET | B | 430 | -11.787 | 79.431 | 15.689 | 1.00 | 45.34 | 6 |
| | ATOM | 1323 | SD | MET | B | 430 | -10.729 | 80.768 | 15.158 | 1.00 | 52.55 | 16 |
| 40 | ATOM | 1324 | CE | MET | B | 430 | -10.070 | 80.157 | 13.610 | 1.00 | 55.56 | 6 |
| | ATOM | 1325 | C | MET | B | 430 | -14.638 | 80.217 | 13.284 | 1.00 | 34.01 | 6 |
| | ATOM | 1326 | O | MET | B | 430 | -14.395 | 80.996 | 12.385 | 1.00 | 37.29 | 8 |
| | ATOM | 1327 | N | ILE | B | 431 | -15.516 | 79.217 | 13.176 | 1.00 | 29.99 | 7 |
| | ATOM | 1328 | CA | ILE | B | 431 | -16.296 | 78.992 | 11.963 | 1.00 | 28.82 | 6 |
| 45 | ATOM | 1329 | CB | ILE | B | 431 | -17.391 | 77.929 | 12.177 | 1.00 | 27.39 | 6 |
| | ATOM | 1330 | CG2 | ILE | B | 431 | -18.314 | 77.841 | 10.959 | 1.00 | 23.87 | 6 |
| | ATOM | 1331 | CG1 | ILE | B | 431 | -16.784 | 76.555 | 12.449 | 1.00 | 25.56 | 6 |
| | ATOM | 1332 | CD1 | ILE | B | 431 | -17.826 | 75.464 | 12.498 | 1.00 | 17.29 | 6 |
| | ATOM | 1333 | C | ILE | B | 431 | -16.953 | 80.288 | 11.538 | 1.00 | 29.49 | 6 |
| 50 | ATOM | 1334 | O | ILE | B | 431 | -16.837 | 80.725 | 10.398 | 1.00 | 24.19 | 8 |
| | ATOM | 1335 | N | GLY | B | 432 | -17.657 | 80.904 | 12.474 | 1.00 | 25.25 | 7 |
| | ATOM | 1336 | CA | GLY | B | 432 | -18.357 | 82.142 | 12.179 | 1.00 | 30.38 | 6 |
| | ATOM | 1337 | C | GLY | B | 432 | -17.395 | 83.209 | 11.725 | 1.00 | 32.75 | 6 |
| | ATOM | 1338 | O | GLY | B | 432 | -17.531 | 83.740 | 10.637 | 1.00 | 36.38 | 8 |
| 55 | ATOM | 1339 | N | ALA | B | 433 | -16.431 | 83.522 | 12.586 | 1.00 | 26.77 | 7 |
| | ATOM | 1340 | CA | ALA | B | 433 | -15.407 | 84.514 | 12.299 | 1.00 | 26.48 | 6 |
| | ATOM | 1341 | CB | ALA | B | 433 | -14.240 | 84.338 | 13.253 | 1.00 | 19.90 | 6 |
| | ATOM | 1342 | C | ALA | B | 433 | -14.905 | 84.433 | 10.867 | 1.00 | 30.73 | 6 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 1343 | O | ALA | B | 433 | -14.849 | 85.432 | 10.171 | 1.00 | 31.60 | 8 |
| | ATOM | 1344 | N | CYS | B | 434 | -14.534 | 83.246 | 10.439 | 1.00 | 33.22 | 7 |
| | ATOM | 1345 | CA | CYS | B | 434 | -14.023 | 83.021 | 9.120 | 1.00 | 34.34 | 6 |
| | ATOM | 1346 | CB | CYS | B | 434 | -13.553 | 81.661 | 9.226 | 1.00 | 35.20 | 6 |
| | ATOM | 1347 | SG | CYS | B | 434 | -12.412 | 81.249 | 8.444 | 1.00 | 54.48 | 16 |
| 10 | ATOM | 1348 | C | CYS | B | 434 | -15.106 | 83.116 | 8.062 | 1.00 | 34.09 | 6 |
| | ATOM | 1349 | O | CYS | B | 434 | -14.844 | 83.555 | 6.952 | 1.00 | 34.89 | 8 |
| | ATOM | 1350 | N | HIS | B | 435 | -16.318 | 82.699 | 8.394 | 1.00 | 34.30 | 7 |
| | ATOM | 1351 | CA | HIS | B | 435 | -17.395 | 82.762 | 7.443 | 1.00 | 35.44 | 6 |
| | ATOM | 1352 | CB | HIS | B | 435 | -18.700 | 82.404 | 8.103 | 1.00 | 31.76 | 6 |
| 15 | ATOM | 1353 | CG | HIS | B | 435 | -19.845 | 82.425 | 7.149 | 1.00 | 32.03 | 6 |
| | ATOM | 1354 | CD2 | HIS | B | 435 | -20.483 | 81.419 | 6.515 | 1.00 | 28.61 | 6 |
| | ATOM | 1355 | ND1 | HIS | B | 435 | -20.345 | 83.600 | 6.607 | 1.00 | 28.48 | 7 |
| | ATOM | 1356 | CE1 | HIS | B | 435 | -21.241 | 83.293 | 5.672 | 1.00 | 33.27 | 6 |
| | ATOM | 1357 | NE2 | HIS | B | 435 | -21.341 | 81.977 | 5.605 | 1.00 | 31.57 | 7 |
| 20 | ATOM | 1358 | C | HIS | B | 435 | -17.528 | 84.152 | 6.878 | 1.00 | 32.74 | 6 |
| | ATOM | 1359 | O | HIS | B | 435 | -17.842 | 84.326 | 5.715 | 1.00 | 32.87 | 8 |
| | ATOM | 1360 | N | ALA | B | 436 | -17.315 | 85.121 | 7.758 | 1.00 | 31.01 | 7 |
| | ATOM | 1361 | CA | ALA | B | 436 | -17.376 | 86.520 | 7.405 | 1.00 | 29.91 | 6 |
| | ATOM | 1362 | CB | ALA | B | 436 | -17.008 | 87.352 | 8.618 | 1.00 | 21.23 | 6 |
| 25 | ATOM | 1363 | C | ALA | B | 436 | -16.393 | 86.782 | 6.266 | 1.00 | 33.86 | 6 |
| | ATOM | 1364 | O | ALA | B | 436 | -16.734 | 87.398 | 5.257 | 1.00 | 36.10 | 8 |
| | ATOM | 1365 | N | SER | B | 437 | -15.162 | 86.307 | 6.448 | 1.00 | 35.19 | 7 |
| | ATOM | 1366 | CA | SER | B | 437 | -14.122 | 86.484 | 5.445 | 1.00 | 33.03 | 6 |
| | ATOM | 1367 | CB | SER | B | 437 | -12.882 | 85.688 | 5.847 | 1.00 | 35.31 | 6 |
| 30 | ATOM | 1368 | OG | SER | B | 437 | -11.855 | 85.824 | 4.879 | 1.00 | 44.99 | 8 |
| | ATOM | 1369 | C | SER | B | 437 | -14.642 | 85.993 | 4.108 | 1.00 | 38.39 | 6 |
| | ATOM | 1370 | O | SER | B | 437 | -14.700 | 86.730 | 3.127 | 1.00 | 37.54 | 8 |
| | ATOM | 1371 | N | ARG | B | 438 | -15.008 | 84.719 | 4.096 | 1.00 | 37.32 | 7 |
| | ATOM | 1372 | CA | ARG | B | 438 | -15.526 | 84.068 | 2.908 | 1.00 | 39.30 | 6 |
| 35 | ATOM | 1373 | CB | ARG | B | 438 | -16.019 | 82.660 | 3.259 | 1.00 | 42.97 | 6 |
| | ATOM | 1374 | CG | ARG | B | 438 | -14.910 | 81.673 | 3.590 | 1.00 | 41.72 | 6 |
| | ATOM | 1375 | CD | ARG | B | 438 | -14.044 | 81.488 | 2.356 | 1.00 | 45.23 | 6 |
| | ATOM | 1376 | NE | ARG | B | 438 | -14.781 | 80.936 | 1.235 | 1.00 | 45.66 | 7 |
| | ATOM | 1377 | CZ | ARG | B | 438 | -14.482 | 81.175 | -0.040 | 1.00 | 49.71 | 6 |
| 40 | ATOM | 1378 | NH1 | ARG | B | 438 | -13.458 | 81.977 | -0.347 | 1.00 | 50.91 | 7 |
| | ATOM | 1379 | NH2 | ARG | B | 438 | -15.219 | 80.619 | -1.002 | 1.00 | 46.86 | 7 |
| | ATOM | 1380 | C | ARG | B | 438 | -16.659 | 84.859 | 2.287 | 1.00 | 42.37 | 6 |
| | ATOM | 1381 | O | ARG | B | 438 | -16.841 | 84.832 | 1.072 | 1.00 | 40.58 | 8 |
| | ATOM | 1382 | N | PHE | B | 439 | -17.417 | 85.575 | 3.117 | 1.00 | 42.25 | 7 |
| 45 | ATOM | 1383 | CA | PHE | B | 439 | -18.531 | 86.354 | 2.614 | 1.00 | 42.81 | 6 |
| | ATOM | 1384 | CB | PHE | B | 439 | -19.198 | 87.132 | 3.731 | 1.00 | 42.18 | 6 |
| | ATOM | 1385 | CG | PHE | B | 439 | -20.487 | 87.769 | 3.323 | 1.00 | 42.48 | 6 |
| | ATOM | 1386 | CD1 | PHE | B | 439 | -21.535 | 86.981 | 2.912 | 1.00 | 47.09 | 6 |
| | ATOM | 1387 | CD2 | PHE | B | 439 | -20.638 | 89.141 | 3.334 | 1.00 | 39.76 | 6 |
| 50 | ATOM | 1388 | CE1 | PHE | B | 439 | -22.735 | 87.543 | 2.527 | 1.00 | 49.17 | 6 |
| | ATOM | 1389 | CE2 | PHE | B | 439 | -21.851 | 89.717 | 2.944 | 1.00 | 45.10 | 6 |
| | ATOM | 1390 | CZ | PHE | B | 439 | -22.901 | 88.911 | 2.538 | 1.00 | 46.36 | 6 |
| | ATOM | 1391 | C | PHE | B | 439 | -18.016 | 87.319 | 1.581 | 1.00 | 44.79 | 6 |
| | ATOM | 1392 | O | PHE | B | 439 | -18.514 | 87.354 | 0.465 | 1.00 | 40.26 | 8 |
| 55 | ATOM | 1393 | N | LEU | B | 440 | -17.021 | 88.117 | 1.987 | 1.00 | 42.77 | 7 |
| | ATOM | 1394 | CA | LEU | B | 440 | -16.415 | 89.115 | 1.109 | 1.00 | 42.96 | 6 |
| | ATOM | 1395 | CB | LEU | B | 440 | -15.169 | 89.718 | 1.768 | 1.00 | 37.19 | 6 |
| | ATOM | 1396 | CG | LEU | B | 440 | -15.477 | 90.588 | 2.967 | 1.00 | 36.97 | 6 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 1397 | CD1 | LEU | B | 440 | -14.219 | 91.352 | 3.402 | 1.00 | 33.65 | 6 |
| | ATOM | 1398 | CD2 | LEU | B | 440 | -16.577 | 91.591 | 2.574 | 1.00 | 35.42 | 6 |
| | ATOM | 1399 | C | LEU | B | 440 | -16.099 | 88.561 | -0.273 | 1.00 | 45.47 | 6 |
| | ATOM | 1400 | O | LEU | B | 440 | -16.631 | 89.059 | -1.265 | 1.00 | 52.48 | 8 |
| | ATOM | 1401 | N | HIS | B | 441 | -15.238 | 87.549 | -0.345 | 1.00 | 49.15 | 7 |
| 10 | ATOM | 1402 | CA | HIS | B | 441 | -14.929 | 86.956 | -1.632 | 1.00 | 54.76 | 6 |
| | ATOM | 1403 | CB | HIS | B | 441 | -14.150 | 85.700 | -1.448 | 1.00 | 56.68 | 6 |
| | ATOM | 1404 | CG | HIS | B | 441 | -12.713 | 85.934 | -1.230 | 1.00 | 62.73 | 6 |
| | ATOM | 1405 | CD2 | HIS | B | 441 | -11.602 | 85.418 | -1.812 | 1.00 | 65.73 | 6 |
| | ATOM | 1406 | ND1 | HIS | B | 441 | -12.245 | 86.850 | -0.273 | 1.00 | 66.01 | 7 |
| 15 | ATOM | 1407 | CE1 | HIS | B | 441 | -10.916 | 86.847 | -0.309 | 1.00 | 65.55 | 6 |
| | ATOM | 1408 | NE2 | HIS | B | 441 | -10.512 | 85.993 | -1.228 | 1.00 | 60.09 | 7 |
| | ATOM | 1409 | C | HIS | B | 441 | -16.217 | 86.633 | -2.301 | 1.00 | 55.93 | 6 |
| | ATOM | 1410 | O | HIS | B | 441 | -16.418 | 86.938 | -3.465 | 1.00 | 57.33 | 8 |
| | ATOM | 1411 | N | MET | B | 442 | -17.106 | 85.997 | -1.553 | 1.00 | 57.81 | 7 |
| 20 | ATOM | 1412 | CA | MET | B | 442 | -18.399 | 85.652 | -2.106 | 1.00 | 59.11 | 6 |
| | ATOM | 1413 | CB | MET | B | 442 | -19.340 | 85.162 | -1.008 | 1.00 | 55.93 | 6 |
| | ATOM | 1414 | CG | MET | B | 442 | -18.991 | 83.796 | -0.456 | 1.00 | 58.52 | 6 |
| | ATOM | 1415 | SD | MET | B | 442 | -20.310 | 82.994 | 0.505 | 1.00 | 60.99 | 16 |
| | ATOM | 1416 | CE | MET | B | 442 | -20.525 | 84.203 | 1.827 | 1.00 | 52.61 | 6 |
| 25 | ATOM | 1417 | C | MET | B | 442 | -18.991 | 86.879 | -2.785 | 1.00 | 60.31 | 6 |
| | ATOM | 1418 | O | MET | B | 442 | -19.646 | 86.778 | -3.817 | 1.00 | 58.18 | 8 |
| | ATOM | 1419 | N | LYS | B | 443 | -18.731 | 88.045 | -2.213 | 1.00 | 61.45 | 7 |
| | ATOM | 1420 | CA | LYS | B | 443 | -19.267 | 89.268 | -2.758 | 1.00 | 64.90 | 6 |
| | ATOM | 1421 | CB | LYS | B | 443 | -19.182 | 90.358 | -1.704 | 1.00 | 64.40 | 6 |
| 30 | ATOM | 1422 | CG | LYS | B | 443 | -20.160 | 91.449 | -1.982 | 1.00 | 69.12 | 6 |
| | ATOM | 1423 | CD | LYS | B | 443 | -19.763 | 92.673 | -1.306 | 1.00 | 71.14 | 6 |
| | ATOM | 1424 | CE | LYS | B | 443 | -20.508 | 92.993 | -0.491 | 1.00 | 73.43 | 6 |
| | ATOM | 1425 | NZ | LYS | B | 443 | -20.174 | 94.242 | 0.151 | 1.00 | 67.97 | 7 |
| | ATOM | 1426 | C | LYS | B | 443 | -18.528 | 89.704 | -4.020 | 1.00 | 67.29 | 6 |
| 35 | ATOM | 1427 | O | LYS | B | 443 | -18.979 | 90.586 | -4.731 | 1.00 | 67.90 | 8 |
| | ATOM | 1428 | N | VAL | B | 444 | -17.383 | 89.075 | -4.285 | 1.00 | 66.57 | 7 |
| | ATOM | 1429 | CA | VAL | B | 444 | -16.589 | 89.418 | -5.455 | 1.00 | 64.76 | 6 |
| | ATOM | 1430 | CB | VAL | B | 444 | -15.097 | 89.568 | -5.082 | 1.00 | 62.76 | 6 |
| | ATOM | 1431 | CG1 | VAL | B | 444 | -14.269 | 89.857 | -6.298 | 1.00 | 64.00 | 6 |
| 40 | ATOM | 1432 | CG2 | VAL | B | 444 | -14.905 | 90.678 | -4.042 | 1.00 | 59.27 | 6 |
| | ATOM | 1433 | C | VAL | B | 444 | -16.800 | 88.397 | -6.569 | 1.00 | 68.61 | 6 |
| | ATOM | 1434 | O | VAL | B | 444 | -16.968 | 88.774 | -7.729 | 1.00 | 70.60 | 8 |
| | ATOM | 1435 | N | GLU | B | 445 | -16.812 | 87.118 | -6.219 | 1.00 | 70.71 | 7 |
| | ATOM | 1436 | CA | GLU | B | 445 | -16.951 | 86.033 | -7.197 | 1.00 | 71.45 | 6 |
| 45 | ATOM | 1437 | CB | GLU | B | 445 | -16.169 | 84.809 | -6.712 | 1.00 | 72.36 | 6 |
| | ATOM | 1438 | CG | GLU | B | 445 | -14.736 | 85.090 | -6.392 | 1.00 | 40.00 | 6 |
| | ATOM | 1439 | CD | GLU | B | 445 | -13.998 | 83.890 | -5.851 | 1.00 | 40.00 | 6 |
| | ATOM | 1440 | OE1 | GLU | B | 445 | -14.587 | 82.798 | -5.665 | 1.00 | 40.00 | 8 |
| | ATOM | 1441 | OE2 | GLU | B | 445 | -12.775 | 83.995 | -5.580 | 1.00 | 40.00 | 8 |
| 50 | ATOM | 1442 | C | GLU | B | 445 | -18.375 | 85.574 | -7.422 | 1.00 | 71.46 | 6 |
| | ATOM | 1443 | O | GLU | B | 445 | -18.605 | 84.542 | -8.064 | 1.00 | 73.02 | 8 |
| | ATOM | 1444 | N | CYS | B | 446 | -19.328 | 86.333 | -6.900 | 1.00 | 71.12 | 7 |
| | ATOM | 1445 | CA | CYS | B | 446 | -20.694 | 85.942 | -7.062 | 1.00 | 70.83 | 6 |
| | ATOM | 1446 | CB | CYS | B | 446 | -21.196 | 85.230 | -5.784 | 1.00 | 71.05 | 6 |
| 55 | ATOM | 1447 | SG | CYS | B | 446 | -20.296 | 83.720 | -5.349 | 1.00 | 72.83 | 16 |
| | ATOM | 1448 | C | CYS | B | 446 | -21.563 | 87.135 | -7.386 | 1.00 | 71.91 | 6 |
| | ATOM | 1449 | O | CYS | B | 446 | -21.307 | 88.244 | -6.911 | 1.00 | 72.06 | 8 |
| | ATOM | 1450 | N | PRO | B | 447 | -22.550 | 86.928 | -8.256 | 1.00 | 73.12 | 7 |

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|----|------|------|-----|-----------|---------|--------|---------|------|-------|---|
| 5 | ATOM | 1451 | CD | PRO B 447 | -22.837 | 85.637 | -8.886 | 1.00 | 72.88 | 6 |
| | ATOM | 1452 | CA | PRO B 447 | -23.461 | 87.997 | -8.653 | 1.00 | 74.22 | 6 |
| | ATOM | 1453 | CB | PRO B 447 | -24.399 | 87.338 | -9.659 | 1.00 | 72.98 | 6 |
| | ATOM | 1454 | CG | PRO B 447 | -23.981 | 85.934 | -9.776 | 1.00 | 74.77 | 6 |
| | ATOM | 1455 | C | PRO B 447 | -24.203 | 88.519 | -7.451 | 1.00 | 75.94 | 6 |
| 10 | ATOM | 1456 | O | PRO B 447 | -24.601 | 87.749 | -6.611 | 1.00 | 76.67 | 8 |
| | ATOM | 1457 | N | THR B 448 | -24.390 | 89.828 | -7.373 | 1.00 | 76.91 | 7 |
| | ATOM | 1458 | CA | THR B 448 | -25.134 | 90.436 | -6.268 | 1.00 | 78.24 | 6 |
| | ATOM | 1459 | CB | THR B 448 | -24.883 | 91.948 | -6.276 | 1.00 | 81.33 | 6 |
| | ATOM | 1460 | OG1 | THR B 448 | -25.474 | 92.525 | -7.451 | 1.00 | 84.46 | 8 |
| 15 | ATOM | 1461 | CG2 | THR B 448 | -23.394 | 92.234 | -6.269 | 1.00 | 83.51 | 6 |
| | ATOM | 1462 | C | THR B 448 | -26.594 | 90.160 | -6.619 | 1.00 | 77.42 | 6 |
| | ATOM | 1463 | O | THR B 448 | -27.512 | 90.649 | -5.982 | 1.00 | 77.65 | 8 |
| | ATOM | 1464 | N | GLU B 449 | -26.759 | 89.400 | -7.697 | 1.00 | 76.29 | 7 |
| | ATOM | 1465 | CA | GLU B 449 | -28.051 | 89.017 | -8.211 | 1.00 | 75.03 | 6 |
| 20 | ATOM | 1466 | CB | GLU B 449 | -27.923 | 88.915 | -9.719 | 1.00 | 74.62 | 6 |
| | ATOM | 1467 | CG | GLU B 449 | -28.823 | 87.966 | -10.343 | 1.00 | 40.00 | 6 |
| | ATOM | 1468 | CD | GLU B 449 | -28.522 | 87.831 | -11.756 | 1.00 | 40.00 | 6 |
| | ATOM | 1469 | OE1 | GLU B 449 | -27.366 | 88.072 | -12.190 | 1.00 | 40.00 | 8 |
| | ATOM | 1470 | OE2 | GLU B 449 | -29.449 | 87.438 | -12.492 | 1.00 | 40.00 | 8 |
| 25 | ATOM | 1471 | C | GLU B 449 | -28.448 | 87.660 | -7.609 | 1.00 | 73.49 | 6 |
| | ATOM | 1472 | O | GLU B 449 | -29.479 | 87.092 | -7.953 | 1.00 | 70.24 | 8 |
| | ATOM | 1473 | N | LEU B 450 | -27.624 | 87.158 | -6.695 | 1.00 | 70.80 | 7 |
| | ATOM | 1474 | CA | LEU B 450 | -27.879 | 85.879 | -6.058 | 1.00 | 68.82 | 6 |
| | ATOM | 1475 | CB | LEU B 450 | -26.772 | 84.887 | -6.447 | 1.00 | 71.91 | 6 |
| 30 | ATOM | 1476 | CG | LEU B 450 | -26.612 | 84.503 | -7.900 | 1.00 | 76.62 | 6 |
| | ATOM | 1477 | CD1 | LEU B 450 | -25.396 | 83.637 | -8.059 | 1.00 | 77.95 | 6 |
| | ATOM | 1478 | CD2 | LEU B 450 | -27.849 | 83.775 | -8.351 | 1.00 | 76.46 | 6 |
| | ATOM | 1479 | C | LEU B 450 | -27.941 | 86.012 | -4.536 | 1.00 | 66.22 | 6 |
| | ATOM | 1480 | O | LEU B 450 | -28.251 | 85.039 | -3.849 | 1.00 | 66.01 | 8 |
| 35 | ATOM | 1481 | N | PHE B 451 | -27.666 | 87.215 | -4.012 | 1.00 | 61.96 | 7 |
| | ATOM | 1482 | CA | PHE B 451 | -27.635 | 87.494 | -2.585 | 1.00 | 58.44 | 6 |
| | ATOM | 1483 | CB | PHE B 451 | -26.579 | 88.573 | -2.263 | 1.00 | 61.34 | 6 |
| | ATOM | 1484 | CG | PHE B 451 | -25.153 | 88.078 | -2.413 | 1.00 | 63.02 | 6 |
| | ATOM | 1485 | CD1 | PHE B 451 | -24.675 | 87.587 | -3.626 | 1.00 | 62.92 | 6 |
| 40 | ATOM | 1486 | CD2 | PHE B 451 | -24.283 | 88.173 | -1.346 | 1.00 | 63.07 | 6 |
| | ATOM | 1487 | CE1 | PHE B 451 | -23.327 | 87.217 | -3.757 | 1.00 | 65.12 | 6 |
| | ATOM | 1488 | CE2 | PHE B 451 | -22.939 | 87.806 | -1.472 | 1.00 | 64.66 | 6 |
| | ATOM | 1489 | CZ | PHE B 451 | -22.459 | 87.335 | -2.686 | 1.00 | 67.12 | 6 |
| | ATOM | 1490 | C | PHE B 451 | -28.931 | 87.994 | -1.962 | 1.00 | 56.41 | 6 |
| 45 | ATOM | 1491 | O | PHE B 451 | -29.207 | 89.214 | -1.908 | 1.00 | 56.56 | 8 |
| | ATOM | 1492 | N | PRO B 452 | -29.791 | 87.072 | -1.473 | 1.00 | 53.28 | 7 |
| | ATOM | 1493 | CD | PRO B 452 | -29.767 | 85.611 | -1.494 | 1.00 | 50.46 | 6 |
| | ATOM | 1494 | CA | PRO B 452 | -31.037 | 87.598 | -0.843 | 1.00 | 50.26 | 6 |
| | ATOM | 1495 | CB | PRO B 452 | -31.746 | 86.375 | -0.301 | 1.00 | 49.19 | 6 |
| 50 | ATOM | 1496 | CG | PRO B 452 | -31.024 | 85.197 | -0.842 | 1.00 | 45.89 | 6 |
| | ATOM | 1497 | C | PRO B 452 | -30.636 | 88.567 | 0.251 | 1.00 | 49.62 | 6 |
| | ATOM | 1498 | O | PRO B 452 | -29.628 | 88.401 | 0.906 | 1.00 | 52.35 | 8 |
| | ATOM | 1499 | N | PRO B 453 | -31.494 | 89.539 | 0.535 | 1.00 | 51.50 | 7 |
| | ATOM | 1500 | CD | PRO B 453 | -32.853 | 89.644 | 0.022 | 1.00 | 49.66 | 6 |
| 55 | ATOM | 1501 | CA | PRO B 453 | -31.184 | 90.573 | 1.530 | 1.00 | 50.89 | 6 |
| | ATOM | 1502 | CB | PRO B 453 | -32.422 | 91.401 | 1.625 | 1.00 | 51.49 | 6 |
| | ATOM | 1503 | CG | PRO B 453 | -33.378 | 90.827 | 0.724 | 1.00 | 50.82 | 6 |
| | ATOM | 1504 | C | PRO B 453 | -30.829 | 90.039 | 2.906 | 1.00 | 50.99 | 6 |

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|----|------|------|-----|-----------|---------|--------|--------|------|-------|---|
| 5 | ATOM | 1505 | O | PRO B 453 | -29.700 | 90.206 | 3.345 | 1.00 | 54.17 | 8 |
| | ATOM | 1506 | N | LEU B 454 | -31.807 | 89.458 | 3.631 | 1.00 | 51.21 | 7 |
| | ATOM | 1507 | CA | LEU B 454 | -31.538 | 88.945 | 4.948 | 1.00 | 47.17 | 6 |
| | ATOM | 1508 | CB | LEU B 454 | -32.550 | 87.858 | 5.330 | 1.00 | 44.44 | 6 |
| | ATOM | 1509 | CG | LEU B 454 | -32.347 | 87.412 | 6.748 | 1.00 | 41.33 | 6 |
| 10 | ATOM | 1510 | CD1 | LEU B 454 | -31.987 | 88.589 | 7.631 | 1.00 | 35.93 | 6 |
| | ATOM | 1511 | CD2 | LEU B 454 | -33.590 | 86.732 | 7.239 | 1.00 | 34.79 | 6 |
| | ATOM | 1512 | C | LEU B 454 | -30.099 | 88.443 | 4.928 | 1.00 | 42.25 | 6 |
| | ATOM | 1513 | O | LEU B 454 | -29.323 | 88.774 | 5.812 | 1.00 | 40.82 | 8 |
| | ATOM | 1514 | N | PHE B 455 | -29.716 | 87.707 | 3.885 | 1.00 | 39.29 | 7 |
| 15 | ATOM | 1515 | CA | PHE B 455 | -28.347 | 87.204 | 3.770 | 1.00 | 41.81 | 6 |
| | ATOM | 1516 | CB | PHE B 455 | -28.132 | 86.536 | 2.418 | 1.00 | 47.22 | 6 |
| | ATOM | 1517 | CG | PHE B 455 | -26.813 | 85.836 | 2.292 | 1.00 | 56.97 | 6 |
| | ATOM | 1518 | CD1 | PHE B 455 | -26.437 | 84.915 | 3.247 | 1.00 | 57.23 | 6 |
| | ATOM | 1519 | CD2 | PHE B 455 | -25.949 | 86.094 | 1.236 | 1.00 | 59.40 | 6 |
| 20 | ATOM | 1520 | CE1 | PHE B 455 | -25.225 | 84.234 | 3.153 | 1.00 | 56.58 | 6 |
| | ATOM | 1521 | CE2 | PHE B 455 | -24.720 | 85.409 | 1.134 | 1.00 | 61.80 | 6 |
| | ATOM | 1522 | CZ | PHE B 455 | -24.360 | 84.481 | 2.103 | 1.00 | 59.94 | 6 |
| | ATOM | 1523 | C | PHE B 455 | -27.400 | 88.386 | 3.923 | 1.00 | 45.12 | 6 |
| | ATOM | 1524 | O | PHE B 455 | -26.657 | 88.450 | 4.889 | 1.00 | 39.95 | 8 |
| 25 | ATOM | 1525 | N | LEU B 456 | -27.439 | 89.303 | 2.949 | 1.00 | 43.92 | 7 |
| | ATOM | 1526 | CA | LEU B 456 | -26.597 | 90.503 | 2.947 | 1.00 | 44.08 | 6 |
| | ATOM | 1527 | CB | LEU B 456 | -27.001 | 91.440 | 1.802 | 1.00 | 50.20 | 6 |
| | ATOM | 1528 | CG | LEU B 456 | -26.439 | 91.155 | 0.432 | 1.00 | 55.79 | 6 |
| | ATOM | 1529 | CD1 | LEU B 456 | -27.064 | 92.082 | -0.591 | 1.00 | 54.70 | 6 |
| 30 | ATOM | 1530 | CD2 | LEU B 456 | -24.920 | 91.345 | 0.494 | 1.00 | 53.01 | 6 |
| | ATOM | 1531 | C | LEU B 456 | -26.689 | 91.245 | 4.264 | 1.00 | 44.65 | 6 |
| | ATOM | 1532 | O | LEU B 456 | -25.678 | 91.540 | 4.886 | 1.00 | 45.93 | 8 |
| | ATOM | 1533 | N | GLU B 457 | -27.990 | 91.268 | 4.265 | 1.00 | 44.56 | 7 |
| | ATOM | 1534 | CA | GLU B 457 | -28.288 | 92.016 | 5.497 | 1.00 | 46.37 | 6 |
| 35 | ATOM | 1535 | C | GLU B 457 | -27.434 | 91.452 | 6.628 | 1.00 | 43.60 | 6 |
| | ATOM | 1536 | O | GLU B 457 | -26.754 | 92.223 | 7.339 | 1.00 | 42.69 | 8 |
| | ATOM | 1537 | CB | GLU B 457 | -29.769 | 91.879 | 5.855 | 1.00 | 50.16 | 6 |
| | ATOM | 1538 | CG | GLU B 457 | -30.208 | 92.849 | 6.954 | 1.00 | 20.00 | 6 |
| | ATOM | 1539 | CD | GLU B 457 | -31.646 | 93.338 | 6.782 | 1.00 | 20.00 | 6 |
| 40 | ATOM | 1540 | OE1 | GLU B 457 | -32.351 | 92.932 | 5.779 | 1.00 | 20.00 | 8 |
| | ATOM | 1541 | OE2 | GLU B 457 | -32.157 | 94.156 | 7.638 | 1.00 | 20.00 | 8 |
| | ATOM | 1542 | N | VAL B 458 | -27.428 | 90.413 | 7.281 | 1.00 | 43.21 | 7 |
| | ATOM | 1543 | CA | VAL B 458 | -26.706 | 89.739 | 8.351 | 1.00 | 44.98 | 6 |
| | ATOM | 1544 | CB | VAL B 458 | -27.075 | 88.255 | 8.432 | 1.00 | 44.83 | 6 |
| 45 | ATOM | 1545 | CG1 | VAL B 458 | -26.440 | 87.623 | 9.646 | 1.00 | 49.72 | 6 |
| | ATOM | 1546 | CG2 | VAL B 458 | -28.562 | 88.086 | 8.474 | 1.00 | 40.89 | 6 |
| | ATOM | 1547 | C | VAL B 458 | -25.190 | 89.822 | 8.311 | 1.00 | 42.72 | 6 |
| | ATOM | 1548 | O | VAL B 458 | -24.551 | 90.179 | 9.303 | 1.00 | 42.88 | 8 |
| | ATOM | 1549 | N | PHE B 459 | -24.605 | 89.488 | 7.180 | 1.00 | 44.53 | 7 |
| 50 | ATOM | 1550 | CA | PHE B 459 | -23.165 | 89.480 | 7.077 | 1.00 | 48.18 | 6 |
| | ATOM | 1551 | CB | PHE B 459 | -22.747 | 88.457 | 6.065 | 1.00 | 43.60 | 6 |
| | ATOM | 1552 | CG | PHE B 459 | -23.167 | 87.116 | 6.441 | 1.00 | 40.79 | 6 |
| | ATOM | 1553 | CD1 | PHE B 459 | -24.494 | 86.750 | 6.368 | 1.00 | 41.01 | 6 |
| | ATOM | 1554 | CD2 | PHE B 459 | -22.263 | 86.286 | 7.009 | 1.00 | 39.48 | 6 |
| 55 | ATOM | 1555 | CE1 | PHE B 459 | -24.892 | 85.540 | 6.889 | 1.00 | 40.62 | 6 |
| | ATOM | 1556 | CE2 | PHE B 459 | -22.649 | 85.091 | 7.527 | 1.00 | 36.87 | 6 |
| | ATOM | 1557 | CZ | PHE B 459 | -23.967 | 84.711 | 7.455 | 1.00 | 36.39 | 6 |
| | ATOM | 1558 | C | PHE B 459 | -22.627 | 90.758 | 6.623 | 1.00 | 52.71 | 6 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 1559 | O | PHE | B | 459 | -21.414 | 91.050 | 6.791 | 1.00 | 51.34 | 8 |
| | ATOM | 1560 | N | GLU | B | 460 | -23.489 | 91.531 | 5.976 | 1.00 | 62.92 | 7 |
| | ATOM | 1561 | CA | GLU | B | 460 | -22.953 | 92.741 | 5.533 | 1.00 | 69.33 | 6 |
| | ATOM | 1562 | CB | GLU | B | 460 | -23.851 | 93.487 | 4.505 | 1.00 | 72.95 | 6 |
| | ATOM | 1563 | CG | GLU | B | 460 | -22.917 | 94.002 | 3.412 | 1.00 | 78.35 | 6 |
| 10 | ATOM | 1564 | CD | GLU | B | 460 | -22.908 | 95.480 | 3.256 | 1.00 | 82.97 | 6 |
| | ATOM | 1565 | OE1 | GLU | B | 460 | -23.257 | 96.213 | 4.217 | 1.00 | 88.28 | 8 |
| | ATOM | 1566 | OE2 | GLU | B | 460 | -22.524 | 95.977 | 2.167 | 1.00 | 84.80 | 8 |
| | ATOM | 1567 | C | GLU | B | 460 | -22.790 | 93.576 | 6.786 | 1.00 | 71.87 | 6 |
| | ATOM | 1568 | O | GLU | B | 460 | -23.471 | 93.391 | 7.802 | 1.00 | 74.51 | 8 |
| 15 | ATOM | 1569 | N | ASP | B | 461 | -21.796 | 94.449 | 6.696 | 1.00 | 78.50 | 7 |
| | ATOM | 1570 | CA | ASP | B | 461 | -21.401 | 95.328 | 7.701 | 1.00 | 84.19 | 6 |
| | ATOM | 1571 | CB | ASP | B | 461 | -20.182 | 96.032 | 7.125 | 1.00 | 85.82 | 6 |
| | ATOM | 1572 | CG | ASP | B | 461 | -19.261 | 95.066 | 6.463 | 1.00 | 89.62 | 6 |
| | ATOM | 1573 | OD1 | ASP | B | 461 | -19.670 | 93.929 | 5.982 | 1.00 | 93.00 | 8 |
| 20 | ATOM | 1574 | OD2 | ASP | B | 461 | -18.084 | 95.361 | 6.387 | 1.00 | 93.04 | 8 |
| | ATOM | 1575 | C | ASP | B | 461 | -22.540 | 96.291 | 8.012 | 1.00 | 86.80 | 6 |
| | ATOM | 1576 | O | ASP | B | 461 | -23.063 | 96.176 | 9.139 | 1.00 | 88.70 | 8 |
| | ATOM | 1577 | OXT | ASP | B | 461 | -22.962 | 97.048 | 7.098 | 1.00 | 88.70 | 8 |
| | TER | | | | | | | | | | | |
| 25 | ATOM | 4002 | C1 | T3 | J | 1 | 20.152 | 36.643 | 29.561 | 1.00 | 22.34 | 6 |
| | ATOM | 4003 | C2 | T3 | J | 1 | 19.021 | 41.567 | 29.283 | 1.00 | 21.84 | 6 |
| | ATOM | 4004 | C3 | T3 | J | 1 | 18.880 | 37.086 | 29.226 | 1.00 | 23.43 | 6 |
| | ATOM | 4005 | C4 | T3 | J | 1 | 18.249 | 42.606 | 28.776 | 1.00 | 22.31 | 6 |
| | ATOM | 4006 | C5 | T3 | J | 1 | 18.747 | 38.372 | 28.866 | 1.00 | 24.83 | 6 |
| 30 | ATOM | 4007 | C6 | T3 | J | 1 | 17.938 | 43.621 | 29.664 | 1.00 | 25.16 | 6 |
| | ATOM | 4008 | C7 | T3 | J | 1 | 19.799 | 39.296 | 28.753 | 1.00 | 24.65 | 6 |
| | ATOM | 4009 | C8 | T3 | J | 1 | 18.330 | 43.594 | 31.028 | 1.00 | 21.93 | 6 |
| | ATOM | 4010 | C9 | T3 | J | 1 | 21.101 | 38.940 | 29.075 | 1.00 | 25.09 | 6 |
| | ATOM | 4011 | C10 | T3 | J | 1 | 19.063 | 42.558 | 31.465 | 1.00 | 23.66 | 6 |
| 35 | ATOM | 4012 | C11 | T3 | J | 1 | 21.254 | 37.600 | 29.456 | 1.00 | 23.12 | 6 |
| | ATOM | 4013 | C12 | T3 | J | 1 | 19.459 | 41.490 | 30.621 | 1.00 | 19.67 | 6 |
| | ATOM | 4014 | C13 | T3 | J | 1 | 20.370 | 35.228 | 30.075 | 1.00 | 18.97 | 6 |
| | ATOM | 4015 | C15 | T3 | J | 1 | 21.549 | 34.480 | 29.455 | 1.00 | 19.32 | 6 |
| | ATOM | 4016 | C17 | T3 | J | 1 | 21.535 | 33.003 | 29.710 | 1.00 | 19.02 | 6 |
| 40 | ATOM | 4017 | I1 | T3 | J | 1 | 16.898 | 39.029 | 28.661 | 1.00 | 25.29 | 53 |
| | ATOM | 4018 | I2 | T3 | J | 1 | 17.058 | 45.327 | 29.154 | 1.00 | 26.49 | 53 |
| | ATOM | 4019 | I3 | T3 | J | 1 | 22.763 | 40.262 | 29.169 | 1.00 | 25.67 | 53 |
| | ATOM | 4020 | N1 | T3 | J | 1 | 21.800 | 34.859 | 28.024 | 1.00 | 15.12 | 7 |
| | ATOM | 4021 | O1 | T3 | J | 1 | 17.934 | 44.682 | 31.806 | 1.00 | 21.79 | 8 |
| 45 | ATOM | 4022 | O2 | T3 | J | 1 | 19.432 | 40.560 | 28.362 | 1.00 | 22.05 | 8 |
| | ATOM | 4023 | O3 | T3 | J | 1 | 21.911 | 32.260 | 28.776 | 1.00 | 20.38 | 8 |
| | ATOM | 4024 | O4 | T3 | J | 1 | 21.137 | 32.622 | 30.840 | 1.00 | 20.16 | 8 |
| | TER | | | | | | | | | | | |
| | ATOM | 4025 | C1 | T3 | K | 1 | -28.131 | 75.928 | 7.543 | 1.00 | 22.34 | 6 |
| 50 | ATOM | 4026 | C2 | T3 | K | 1 | -24.676 | 77.673 | 4.318 | 1.00 | 21.84 | 6 |
| | ATOM | 4027 | C3 | T3 | K | 1 | -28.490 | 76.351 | 6.201 | 1.00 | 23.43 | 6 |
| | ATOM | 4028 | C4 | T3 | K | 1 | -24.217 | 77.893 | 2.989 | 1.00 | 22.31 | 6 |
| | ATOM | 4029 | C5 | T3 | K | 1 | -27.485 | 76.499 | 5.233 | 1.00 | 24.83 | 6 |
| | ATOM | 4030 | C6 | T3 | K | 1 | -23.545 | 79.124 | 2.700 | 1.00 | 25.16 | 6 |
| 55 | ATOM | 4031 | C7 | T3 | K | 1 | -26.132 | 76.227 | 5.581 | 1.00 | 24.65 | 6 |
| | ATOM | 4032 | C8 | T3 | K | 1 | -23.382 | 80.104 | 3.772 | 1.00 | 21.93 | 6 |
| | ATOM | 4033 | C9 | T3 | K | 1 | -25.685 | 75.833 | 6.855 | 1.00 | 25.09 | 6 |
| | ATOM | 4034 | C10 | T3 | K | 1 | -23.867 | 79.823 | 5.042 | 1.00 | 23.66 | 6 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 4035 | C11 | T3 | K | 1 | -26.708 | 75.670 | 7.834 | 1.00 | 23.12 | 6 |
| | ATOM | 4036 | C12 | T3 | K | 1 | -24.521 | 78.610 | 5.376 | 1.00 | 19.67 | 6 |
| | ATOM | 4037 | C13 | T3 | K | 1 | -29.211 | 75.830 | 8.626 | 1.00 | 18.97 | 6 |
| | ATOM | 4038 | C15 | T3 | K | 1 | -29.181 | 74.567 | 9.488 | 1.00 | 19.32 | 6 |
| | ATOM | 4039 | C17 | T3 | K | 1 | -30.440 | 74.343 | 10.264 | 1.00 | 19.02 | 6 |
| 10 | ATOM | 4040 | I1 | T3 | K | 1 | -27.868 | 77.342 | 3.316 | 1.00 | 25.29 | 53 |
| | ATOM | 4041 | I2 | T3 | K | 1 | -22.732 | 79.619 | 0.850 | 1.00 | 26.49 | 53 |
| | ATOM | 4042 | I3 | T3 | K | 1 | -23.602 | 75.792 | 7.334 | 1.00 | 25.67 | 53 |
| | ATOM | 4043 | N1 | T3 | K | 1 | -28.680 | 73.342 | 8.762 | 1.00 | 15.12 | 7 |
| | ATOM | 4044 | O1 | T3 | K | 1 | -22.742 | 81.265 | 3.443 | 1.00 | 21.79 | 8 |
| 15 | ATOM | 4045 | O2 | T3 | K | 1 | -25.267 | 76.388 | 4.595 | 1.00 | 22.05 | 8 |
| | ATOM | 4046 | O3 | T3 | K | 1 | -30.816 | 73.159 | 10.382 | 1.00 | 20.38 | 8 |
| | ATOM | 4047 | O4 | T3 | K | 1 | -31.028 | 75.359 | 10.729 | 1.00 | 20.16 | 8 |
| | TER | | | | | | | | | | | |
| | ATOM | 1 | C | LYS | X | 686 | 13.868 | 40.176 | 48.888 | 1.00 | 40.00 | 6 |
| 20 | ATOM | 2 | O | LYS | X | 686 | 13.914 | 40.120 | 47.639 | 1.00 | 40.00 | 8 |
| | ATOM | 3 | N | LYS | X | 686 | 14.374 | 42.245 | 50.489 | 1.00 | 40.00 | 7 |
| | ATOM | 4 | CA | LYS | X | 686 | 14.937 | 41.070 | 49.710 | 1.00 | 40.00 | 6 |
| | ATOM | 5 | N | HIS | X | 687 | 13.038 | 39.527 | 49.705 | 1.00 | 40.00 | 7 |
| | ATOM | 6 | CA | HIS | X | 687 | 11.891 | 38.518 | 49.521 | 1.00 | 40.00 | 6 |
| 25 | ATOM | 7 | CB | HIS | X | 687 | 10.639 | 39.000 | 50.212 | 1.00 | 40.00 | 6 |
| | ATOM | 8 | CG | HIS | X | 687 | 10.981 | 39.526 | 51.563 | 1.00 | 40.00 | 6 |
| | ATOM | 9 | CD2 | HIS | X | 687 | 11.021 | 38.908 | 52.753 | 1.00 | 40.00 | 6 |
| | ATOM | 10 | ND1 | HIS | X | 687 | 11.354 | 40.844 | 51.754 | 1.00 | 40.00 | 7 |
| | ATOM | 11 | CE1 | HIS | X | 687 | 11.614 | 40.994 | 53.034 | 1.00 | 40.00 | 6 |
| 30 | ATOM | 12 | NE2 | HIS | X | 687 | 11.422 | 39.847 | 53.646 | 1.00 | 40.00 | 7 |
| | ATOM | 13 | C | HIS | X | 687 | 11.183 | 38.108 | 48.208 | 1.00 | 40.00 | 6 |
| | ATOM | 14 | O | HIS | X | 687 | 11.674 | 38.361 | 47.094 | 1.00 | 40.00 | 8 |
| | ATOM | 15 | N | LYS | X | 688 | 10.064 | 37.458 | 48.649 | 1.00 | 40.00 | 7 |
| | ATOM | 16 | CA | LYS | X | 688 | 8.911 | 36.858 | 47.931 | 1.00 | 40.00 | 6 |
| 35 | ATOM | 17 | CB | LYS | X | 688 | 8.292 | 37.850 | 46.968 | 1.00 | 40.00 | 6 |
| | ATOM | 18 | C | LYS | X | 688 | 9.246 | 35.573 | 47.161 | 1.00 | 40.00 | 6 |
| | ATOM | 19 | O | LYS | X | 688 | 9.319 | 34.473 | 47.722 | 1.00 | 40.00 | 8 |
| | ATOM | 20 | N | ILE | X | 689 | 9.426 | 35.754 | 45.865 | 1.00 | 40.00 | 7 |
| | ATOM | 21 | CA | ILE | X | 689 | 9.661 | 34.640 | 44.924 | 1.00 | 40.00 | 6 |
| 40 | ATOM | 22 | CB | ILE | X | 689 | 9.731 | 35.167 | 43.498 | 1.00 | 40.00 | 6 |
| | ATOM | 23 | CG2 | ILE | X | 689 | 9.638 | 34.053 | 42.453 | 1.00 | 40.00 | 6 |
| | ATOM | 24 | CG1 | ILE | X | 689 | 8.597 | 36.141 | 43.176 | 1.00 | 40.00 | 6 |
| | ATOM | 25 | CD1 | ILE | X | 689 | 8.250 | 36.183 | 41.688 | 1.00 | 40.00 | 6 |
| | ATOM | 26 | C | ILE | X | 689 | 10.954 | 33.869 | 45.228 | 1.00 | 40.00 | 6 |
| 45 | ATOM | 27 | O | ILE | X | 689 | 10.920 | 32.657 | 45.511 | 1.00 | 40.00 | 8 |
| | ATOM | 28 | N | LEU | X | 690 | 12.065 | 34.579 | 45.140 | 1.00 | 40.00 | 7 |
| | ATOM | 29 | CA | LEU | X | 690 | 13.391 | 33.996 | 45.397 | 1.00 | 40.00 | 6 |
| | ATOM | 30 | CB | LEU | X | 690 | 14.349 | 35.043 | 45.892 | 1.00 | 40.00 | 6 |
| | ATOM | 31 | CG | LEU | X | 690 | 14.450 | 36.168 | 44.906 | 1.00 | 40.00 | 6 |
| 50 | ATOM | 32 | CD1 | LEU | X | 690 | 15.397 | 37.261 | 45.363 | 1.00 | 40.00 | 6 |
| | ATOM | 33 | CD2 | LEU | X | 690 | 14.940 | 35.695 | 43.540 | 1.00 | 40.00 | 6 |
| | ATOM | 34 | C | LEU | X | 690 | 13.271 | 32.999 | 46.466 | 1.00 | 40.00 | 6 |
| | ATOM | 35 | O | LEU | X | 690 | 13.633 | 31.832 | 46.315 | 1.00 | 40.00 | 8 |
| | ATOM | 36 | N | HIS | X | 691 | 12.773 | 33.472 | 47.541 | 1.00 | 40.00 | 7 |
| 55 | ATOM | 37 | CA | HIS | X | 691 | 12.557 | 32.559 | 48.569 | 1.00 | 40.00 | 6 |
| | ATOM | 38 | CB | HIS | X | 691 | 11.729 | 33.212 | 49.658 | 1.00 | 40.00 | 6 |
| | ATOM | 39 | CG | HIS | X | 691 | 12.588 | 34.116 | 50.564 | 1.00 | 40.00 | 6 |
| | ATOM | 40 | CD2 | HIS | X | 691 | 13.648 | 33.852 | 51.385 | 1.00 | 40.00 | 6 |

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|----|------|----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 41 | ND1 | HIS | X | 691 | 12.359 | 35.484 | 50.669 | 1.00 | 40.00 | 7 |
| | ATOM | 42 | CE1 | HIS | X | 691 | 13.242 | 35.991 | 51.513 | 1.00 | 40.00 | 6 |
| | ATOM | 43 | NE2 | HIS | X | 691 | 14.016 | 35.031 | 51.949 | 1.00 | 40.00 | 7 |
| | ATOM | 44 | C | HIS | X | 691 | 11.954 | 31.331 | 47.861 | 1.00 | 40.00 | 6 |
| | ATOM | 45 | O | HIS | X | 691 | 12.505 | 30.240 | 47.882 | 1.00 | 40.00 | 8 |
| 10 | ATOM | 46 | N | ARG | X | 692 | 10.839 | 31.494 | 47.167 | 1.00 | 40.00 | 7 |
| | ATOM | 47 | CA | ARG | X | 692 | 10.169 | 30.333 | 46.518 | 1.00 | 40.00 | 6 |
| | ATOM | 48 | CB | ARG | X | 692 | 9.118 | 30.800 | 45.517 | 1.00 | 40.00 | 6 |
| | ATOM | 49 | C | ARG | X | 692 | 11.153 | 29.402 | 45.752 | 1.00 | 40.00 | 6 |
| | ATOM | 50 | O | ARG | X | 692 | 11.030 | 28.168 | 45.779 | 1.00 | 40.00 | 8 |
| 15 | ATOM | 51 | N | LEU | X | 693 | 12.117 | 30.000 | 45.072 | 1.00 | 40.00 | 7 |
| | ATOM | 52 | CA | LEU | X | 693 | 13.078 | 29.252 | 44.226 | 1.00 | 40.00 | 6 |
| | ATOM | 53 | CB | LEU | X | 693 | 13.784 | 30.210 | 43.274 | 1.00 | 40.00 | 6 |
| | ATOM | 54 | CG | LEU | X | 693 | 12.796 | 31.012 | 42.432 | 1.00 | 40.00 | 6 |
| | ATOM | 55 | CD1 | LEU | X | 693 | 13.479 | 31.969 | 41.458 | 1.00 | 40.00 | 6 |
| 20 | ATOM | 56 | CD2 | LEU | X | 693 | 11.884 | 30.126 | 41.579 | 1.00 | 40.00 | 6 |
| | ATOM | 57 | C | LEU | X | 693 | 14.143 | 28.531 | 45.054 | 1.00 | 40.00 | 6 |
| | ATOM | 58 | O | LEU | X | 693 | 14.702 | 27.508 | 44.633 | 1.00 | 40.00 | 8 |
| | ATOM | 59 | N | LEU | X | 694 | 14.400 | 29.079 | 46.209 | 1.00 | 40.00 | 7 |
| | ATOM | 60 | CA | LEU | X | 694 | 15.407 | 28.538 | 47.115 | 1.00 | 40.00 | 6 |
| 25 | ATOM | 61 | CB | LEU | X | 694 | 15.871 | 29.626 | 48.084 | 1.00 | 40.00 | 6 |
| | ATOM | 62 | CG | LEU | X | 694 | 16.692 | 30.716 | 47.404 | 1.00 | 40.00 | 6 |
| | ATOM | 63 | CD1 | LEU | X | 694 | 17.279 | 31.724 | 48.391 | 1.00 | 40.00 | 6 |
| | ATOM | 64 | CD2 | LEU | X | 694 | 17.879 | 30.156 | 46.619 | 1.00 | 40.00 | 6 |
| | ATOM | 65 | C | LEU | X | 694 | 14.837 | 27.404 | 47.957 | 1.00 | 40.00 | 6 |
| 30 | ATOM | 66 | O | LEU | X | 694 | 15.555 | 26.747 | 48.716 | 1.00 | 40.00 | 8 |
| | ATOM | 67 | N | GLN | X | 695 | 13.554 | 27.157 | 47.809 | 1.00 | 40.00 | 7 |
| | ATOM | 68 | CA | GLN | X | 695 | 12.883 | 26.188 | 48.685 | 1.00 | 40.00 | 6 |
| | ATOM | 69 | C | GLN | X | 695 | 12.423 | 24.910 | 47.977 | 1.00 | 40.00 | 6 |
| | ATOM | 70 | O | GLN | X | 695 | 12.309 | 23.845 | 48.598 | 1.00 | 40.00 | 8 |
| 35 | ATOM | 71 | CB | GLN | X | 695 | 11.681 | 26.858 | 49.322 | 1.00 | 40.00 | 6 |
| | ATOM | 72 | CG | GLN | X | 695 | 12.074 | 28.125 | 50.080 | 1.00 | 20.00 | 6 |
| | ATOM | 73 | CD | GLN | X | 695 | 10.899 | 28.768 | 50.801 | 1.00 | 20.00 | 6 |
| | ATOM | 74 | OE1 | GLN | X | 695 | 9.772 | 28.296 | 50.671 | 1.00 | 20.00 | 8 |
| | ATOM | 75 | NE2 | GLN | X | 695 | 11.092 | 29.828 | 51.560 | 1.00 | 20.00 | 7 |
| 40 | ATOM | 76 | N | ASP | X | 696 | 12.155 | 25.020 | 46.714 | 1.00 | 40.00 | 7 |
| | ATOM | 77 | CA | ASP | X | 696 | 11.698 | 23.885 | 45.910 | 1.00 | 40.00 | 6 |
| | ATOM | 78 | CB | ASP | X | 696 | 11.450 | 24.400 | 44.497 | 1.00 | 40.00 | 6 |
| | ATOM | 79 | CG | ASP | X | 696 | 10.782 | 23.411 | 43.548 | 1.00 | 40.00 | 6 |
| | ATOM | 80 | OD1 | ASP | X | 696 | 10.550 | 22.203 | 43.920 | 1.00 | 40.00 | 8 |
| 45 | ATOM | 81 | OD2 | ASP | X | 696 | 10.449 | 23.804 | 42.362 | 1.00 | 40.00 | 8 |
| | ATOM | 82 | C | ASP | X | 696 | 12.774 | 22.806 | 45.876 | 1.00 | 40.00 | 6 |
| | ATOM | 83 | O | ASP | X | 696 | 13.937 | 23.077 | 45.562 | 1.00 | 40.00 | 8 |
| | ATOM | 84 | N | SER | X | 697 | 12.370 | 21.610 | 46.213 | 1.00 | 40.00 | 7 |
| | ATOM | 85 | CA | SER | X | 697 | 13.258 | 20.453 | 46.128 | 1.00 | 40.00 | 6 |
| 50 | ATOM | 86 | CB | SER | X | 697 | 12.685 | 19.371 | 47.049 | 1.00 | 40.00 | 6 |
| | ATOM | 87 | OG | SER | X | 697 | 12.535 | 19.899 | 48.374 | 1.00 | 40.00 | 8 |
| | ATOM | 88 | C | SER | X | 697 | 13.329 | 20.130 | 44.613 | 1.00 | 40.00 | 6 |
| | ATOM | 89 | O | SER | X | 697 | 14.247 | 20.573 | 43.914 | 1.00 | 40.00 | 8 |
| | ATOM | 90 | N | SER | X | 698 | 12.355 | 19.357 | 44.183 | 1.00 | 40.00 | 7 |
| 55 | ATOM | 91 | CA | SER | X | 698 | 11.985 | 19.100 | 42.752 | 1.00 | 40.00 | 6 |
| | ATOM | 92 | CB | SER | X | 698 | 11.693 | 20.417 | 42.036 | 1.00 | 40.00 | 6 |
| | ATOM | 93 | OG | SER | X | 698 | 10.510 | 21.000 | 42.577 | 1.00 | 40.00 | 8 |
| | ATOM | 94 | C | SER | X | 698 | 12.887 | 18.340 | 41.758 | 1.00 | 40.00 | 6 |

| | | | | | | | | | | | |
|----|------|----|-----|-------|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 95 | O | SER X | 698 | 13.253 | 17.158 | 42.026 | 1.00 | 40.00 | 8 |
| | ATOM | 96 | OXT | SER X | 698 | 13.131 | 18.976 | 40.714 | 1.00 | 40.00 | 8 |
| | TER | | | | | | | | | | |
| | ATOM | 1 | CB | LYS Y | 688 | -33.793 | 96.885 | 6.491 | 1.00 | 40.00 | 6 |
| | ATOM | 2 | C | LYS Y | 688 | -35.002 | 95.370 | 8.130 | 1.00 | 40.00 | 6 |
| 10 | ATOM | 3 | O | LYS Y | 688 | -36.027 | 95.520 | 8.779 | 1.00 | 40.00 | 8 |
| | ATOM | 4 | N | LYS Y | 688 | -32.717 | 96.619 | 8.695 | 1.00 | 40.00 | 7 |
| | ATOM | 5 | CA | LYS Y | 688 | -34.040 | 96.591 | 7.954 | 1.00 | 40.00 | 6 |
| | ATOM | 6 | N | ILE Y | 689 | -34.578 | 93.781 | 6.908 | 1.00 | 40.00 | 7 |
| | ATOM | 7 | CA | ILE Y | 689 | -35.862 | 93.106 | 7.268 | 1.00 | 40.00 | 6 |
| 15 | ATOM | 8 | CB | ILE Y | 689 | -35.971 | 91.759 | 6.572 | 1.00 | 40.00 | 6 |
| | ATOM | 9 | CG2 | ILE Y | 689 | -37.270 | 91.077 | 6.932 | 1.00 | 40.00 | 6 |
| | ATOM | 10 | CG1 | ILE Y | 689 | -35.917 | 91.937 | 5.062 | 1.00 | 40.00 | 6 |
| | ATOM | 11 | CD1 | ILE Y | 689 | -36.341 | 90.691 | 4.289 | 1.00 | 40.00 | 6 |
| | ATOM | 12 | C | ILE Y | 689 | -36.032 | 92.870 | 8.780 | 1.00 | 40.00 | 6 |
| 20 | ATOM | 13 | O | ILE Y | 689 | -36.913 | 93.446 | 9.442 | 1.00 | 40.00 | 8 |
| | ATOM | 14 | N | LEU Y | 690 | -35.019 | 92.834 | 9.787 | 1.00 | 40.00 | 7 |
| | ATOM | 15 | CA | LEU Y | 690 | -34.956 | 92.320 | 11.163 | 1.00 | 40.00 | 6 |
| | ATOM | 16 | CB | LEU Y | 690 | -33.528 | 92.432 | 11.697 | 1.00 | 40.00 | 6 |
| | ATOM | 17 | CG | LEU Y | 690 | -32.516 | 91.647 | 10.864 | 1.00 | 40.00 | 6 |
| 25 | ATOM | 18 | CD1 | LEU Y | 690 | -31.087 | 91.764 | 11.397 | 1.00 | 40.00 | 6 |
| | ATOM | 19 | CD2 | LEU Y | 690 | -32.819 | 90.148 | 10.812 | 1.00 | 40.00 | 6 |
| | ATOM | 20 | C | LEU Y | 690 | -35.899 | 93.123 | 12.065 | 1.00 | 40.00 | 6 |
| | ATOM | 21 | O | LEU Y | 690 | -36.570 | 92.492 | 12.928 | 1.00 | 40.00 | 8 |
| | ATOM | 22 | N | HIS Y | 691 | -36.039 | 94.731 | 11.373 | 1.00 | 40.00 | 7 |
| 30 | ATOM | 23 | CA | HIS Y | 691 | -36.634 | 94.923 | 12.683 | 1.00 | 40.00 | 6 |
| | ATOM | 24 | CB | HIS Y | 691 | -36.334 | 96.383 | 12.935 | 1.00 | 40.00 | 6 |
| | ATOM | 25 | CG | HIS Y | 691 | -35.610 | 97.153 | 13.078 | 1.00 | 40.00 | 6 |
| | ATOM | 26 | CD2 | HIS Y | 691 | -34.757 | 97.640 | 12.159 | 1.00 | 40.00 | 6 |
| | ATOM | 27 | ND1 | HIS Y | 691 | -35.129 | 97.579 | 14.319 | 1.00 | 40.00 | 7 |
| 35 | ATOM | 28 | CE1 | HIS Y | 691 | -34.039 | 98.290 | 14.122 | 1.00 | 40.00 | 6 |
| | ATOM | 29 | NE2 | HIS Y | 691 | -33.786 | 98.346 | 12.815 | 1.00 | 40.00 | 7 |
| | ATOM | 30 | C | HIS Y | 691 | -37.972 | 94.287 | 12.756 | 1.00 | 40.00 | 6 |
| | ATOM | 31 | O | HIS Y | 691 | -38.240 | 93.417 | 13.545 | 1.00 | 40.00 | 8 |
| | ATOM | 32 | N | ARG Y | 692 | -38.265 | 94.388 | 11.505 | 1.00 | 40.00 | 7 |
| 40 | ATOM | 33 | CA | ARG Y | 692 | -39.577 | 93.869 | 11.276 | 1.00 | 40.00 | 6 |
| | ATOM | 34 | CB | ARG Y | 692 | -39.653 | 93.692 | 9.795 | 1.00 | 40.00 | 6 |
| | ATOM | 35 | CG | ARG Y | 692 | -40.759 | 92.764 | 9.329 | 1.00 | 40.00 | 6 |
| | ATOM | 36 | CD | ARG Y | 692 | -40.618 | 92.422 | 7.848 | 1.00 | 40.00 | 6 |
| | ATOM | 37 | NE | ARG Y | 692 | -41.849 | 92.641 | 7.091 | 1.00 | 40.00 | 7 |
| 45 | ATOM | 38 | CZ | ARG Y | 692 | -41.898 | 92.758 | 5.763 | 1.00 | 40.00 | 6 |
| | ATOM | 39 | NH1 | ARG Y | 692 | -40.784 | 92.695 | 5.024 | 1.00 | 40.00 | 7 |
| | ATOM | 40 | NH2 | ARG Y | 692 | -43.034 | 92.940 | 5.080 | 1.00 | 40.00 | 7 |
| | ATOM | 41 | C | ARG Y | 692 | -39.941 | 92.547 | 11.995 | 1.00 | 40.00 | 6 |
| | ATOM | 42 | O | ARG Y | 692 | -41.001 | 92.440 | 12.649 | 1.00 | 40.00 | 8 |
| 50 | ATOM | 43 | N | LEU Y | 693 | -39.095 | 91.576 | 11.816 | 1.00 | 40.00 | 7 |
| | ATOM | 44 | CA | LEU Y | 693 | -39.230 | 90.232 | 12.395 | 1.00 | 40.00 | 6 |
| | ATOM | 45 | CB | LEU Y | 693 | -38.362 | 89.337 | 11.615 | 1.00 | 40.00 | 6 |
| | ATOM | 46 | CG | LEU Y | 693 | -38.737 | 89.375 | 10.132 | 1.00 | 40.00 | 6 |
| | ATOM | 47 | CD1 | LEU Y | 693 | -37.794 | 88.570 | 9.247 | 1.00 | 40.00 | 6 |
| 55 | ATOM | 48 | CD2 | LEU Y | 693 | -40.142 | 88.827 | 9.862 | 1.00 | 40.00 | 6 |
| | ATOM | 49 | C | LEU Y | 693 | -38.921 | 90.378 | 13.816 | 1.00 | 40.00 | 6 |
| | ATOM | 50 | O | LEU Y | 693 | -39.191 | 89.474 | 14.615 | 1.00 | 40.00 | 8 |
| | ATOM | 51 | N | LEU Y | 694 | -38.366 | 91.533 | 14.076 | 1.00 | 40.00 | 7 |

| | | | | | | | | | | | | |
|----|------|----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 52 | CA | LEU | Y | 694 | -38.174 | 91.885 | 15.435 | 1.00 | 40.00 | 6 |
| | ATOM | 53 | CB | LEU | Y | 694 | -37.181 | 93.002 | 15.561 | 1.00 | 40.00 | 6 |
| | ATOM | 54 | CG | LEU | Y | 694 | -35.799 | 92.377 | 15.869 | 1.00 | 40.00 | 6 |
| | ATOM | 55 | CD1 | LEU | Y | 694 | -34.897 | 93.275 | 16.702 | 1.00 | 40.00 | 6 |
| | ATOM | 56 | CD2 | LEU | Y | 694 | -35.897 | 91.055 | 16.661 | 1.00 | 40.00 | 6 |
| 10 | ATOM | 57 | C | LEU | Y | 694 | -39.596 | 91.903 | 15.915 | 1.00 | 40.00 | 6 |
| | ATOM | 58 | O | LEU | Y | 694 | -39.985 | 91.253 | 16.858 | 1.00 | 40.00 | 8 |
| | ATOM | 59 | N | GLN | Y | 695 | -40.787 | 92.229 | 15.048 | 1.00 | 40.00 | 7 |
| | ATOM | 60 | CA | GLN | Y | 695 | -42.034 | 91.457 | 15.543 | 1.00 | 40.00 | 6 |
| | ATOM | 61 | C | GLN | Y | 695 | -43.054 | 90.901 | 14.240 | 1.00 | 40.00 | 6 |
| 15 | ATOM | 62 | O | GLN | Y | 695 | -43.102 | 91.557 | 13.189 | 1.00 | 40.00 | 8 |
| | ATOM | 63 | CB | GLN | Y | 695 | -42.362 | 92.025 | 16.923 | 1.00 | 40.00 | 6 |
| | ATOM | 64 | CG | GLN | Y | 695 | -41.013 | 92.101 | 17.768 | 1.00 | 40.00 | 6 |
| | ATOM | 65 | CD | GLN | Y | 695 | -40.943 | 91.235 | 19.059 | 1.00 | 40.00 | 6 |
| | ATOM | 66 | OE1 | GLN | Y | 695 | -41.828 | 90.426 | 19.318 | 1.00 | 40.00 | 8 |
| 20 | ATOM | 67 | NE2 | GLN | Y | 695 | -39.938 | 91.399 | 19.916 | 1.00 | 40.00 | 7 |
| | ATOM | 68 | N | ASP | Y | 696 | -43.802 | 89.498 | 14.402 | 1.00 | 40.00 | 7 |
| | ATOM | 69 | CA | ASP | Y | 696 | -44.784 | 88.354 | 13.428 | 1.00 | 40.00 | 6 |
| | ATOM | 70 | C | ASP | Y | 696 | -46.034 | 88.934 | 12.759 | 1.00 | 40.00 | 6 |
| | ATOM | 71 | O | ASP | Y | 696 | -46.266 | 88.655 | 11.529 | 1.00 | 40.00 | 8 |
| 25 | ATOM | 72 | CB | ASP | Y | 696 | -45.211 | 87.192 | 14.322 | 1.00 | 40.00 | 6 |
| | ATOM | 73 | CG | ASP | Y | 696 | -44.021 | 86.560 | 15.058 | 1.00 | 40.00 | 6 |
| | ATOM | 74 | OD1 | ASP | Y | 696 | -42.823 | 86.994 | 14.844 | 1.00 | 40.00 | 8 |
| | ATOM | 75 | OD2 | ASP | Y | 696 | -44.212 | 85.591 | 15.889 | 1.00 | 40.00 | 8 |
| 30 | END | | | | | | | | | | | |

5

Appendix 2

Atomic Coordinates for Human ER α Complexed with DES, and a GRIP1 NR-box 2 Peptide

| | | | | | | | | | | |
|----|--------|----------|----------|----------|----------|--------|--------|---------|--------|------------|
| 10 | CRYST1 | 54.094 | 82.217 | 58.041 | 90.00 | 111.33 | 90.00 | P | 21 | 2 |
| | ORIGX1 | 1.000000 | 0.000000 | 0.000000 | 0.000000 | | | | | |
| | ORIGX2 | 0.000000 | 1.000000 | 0.000000 | 0.000000 | | | | | |
| | ORIGX3 | 0.000000 | 0.000000 | 1.000000 | 0.000000 | | | | | |
| | SCALE1 | 0.018486 | 0.000000 | 0.007221 | 0.000000 | | | | | |
| 15 | SCALE2 | 0.000000 | 0.012163 | 0.000000 | 0.000000 | | | | | |
| | SCALE3 | 0.000000 | 0.000000 | 0.018497 | 0.000000 | | | | | |
| | ATOM | 1 | CB | SER | A | 305 | 35.230 | -14.787 | -1.163 | 1.00 73.26 |
| | ATOM | 2 | C | SER | A | 305 | 35.331 | -14.303 | 1.289 | 1.00 72.95 |
| 20 | ATOM | 3 | O | SER | A | 305 | 34.146 | -13.984 | 1.186 | 1.00 72.46 |
| | ATOM | 4 | N | SER | A | 305 | 36.797 | -16.033 | 0.285 | 1.00 74.06 |
| | ATOM | 5 | CA | SER | A | 305 | 36.138 | -14.713 | 0.061 | 1.00 73.59 |
| | ATOM | 6 | N | LEU | A | 306 | 35.982 | -14.313 | 2.449 | 1.00 72.21 |
| | ATOM | 7 | CA | LEU | A | 306 | 35.329 | -13.950 | 3.702 | 1.00 71.05 |
| 25 | ATOM | 8 | CB | LEU | A | 306 | 36.251 | -14.256 | 4.878 | 1.00 70.19 |
| | ATOM | 9 | C | LEU | A | 306 | 34.929 | -12.478 | 3.719 | 1.00 69.57 |
| | ATOM | 10 | O | LEU | A | 306 | 35.580 | -11.638 | 3.100 | 1.00 69.96 |
| | ATOM | 11 | N | ALA | A | 307 | 33.851 | -12.176 | 4.434 | 1.00 68.06 |
| | ATOM | 12 | CA | ALA | A | 307 | 33.358 | -10.810 | 4.541 | 1.00 64.88 |
| 30 | ATOM | 13 | CB | ALA | A | 307 | 31.841 | -10.795 | 4.436 | 1.00 65.83 |
| | ATOM | 14 | C | ALA | A | 307 | 33.792 | -10.204 | 5.866 | 1.00 63.36 |
| | ATOM | 15 | O | ALA | A | 307 | 33.878 | -8.984 | 6.005 | 1.00 62.73 |
| | ATOM | 16 | N | LEU | A | 308 | 34.064 | -11.062 | 6.842 | 1.00 62.52 |
| | ATOM | 17 | CA | LEU | A | 308 | 34.487 | -10.598 | 8.156 | 1.00 62.57 |
| 35 | ATOM | 18 | CB | LEU | A | 308 | 34.423 | -11.745 | 9.171 | 1.00 62.81 |
| | ATOM | 19 | CG | LEU | A | 308 | 33.214 | -12.688 | 9.130 | 1.00 64.21 |
| | ATOM | 20 | CD1 | LEU | A | 308 | 33.188 | -13.513 | 10.406 | 1.00 66.28 |
| | ATOM | 21 | CD2 | LEU | A | 308 | 31.919 | -11.898 | 8.989 | 1.00 63.80 |
| | ATOM | 22 | C | LEU | A | 308 | 35.903 | -10.037 | 8.100 | 1.00 61.61 |
| 40 | ATOM | 23 | O | LEU | A | 308 | 36.385 | -9.445 | 9.066 | 1.00 62.92 |
| | ATOM | 24 | N | SER | A | 309 | 36.561 | -10.219 | 6.959 | 1.00 60.50 |
| | ATOM | 25 | CA | SER | A | 309 | 37.928 | -9.743 | 6.771 | 1.00 58.73 |
| | ATOM | 26 | CB | SER | A | 309 | 38.720 | -10.750 | 5.934 | 1.00 59.53 |
| | ATOM | 27 | OG | SER | A | 309 | 38.889 | -10.283 | 4.606 | 1.00 59.47 |
| 45 | ATOM | 28 | C | SER | A | 309 | 37.986 | -8.373 | 6.099 | 1.00 57.05 |
| | ATOM | 29 | O | SER | A | 309 | 38.965 | -7.637 | 6.249 | 1.00 56.70 |
| | ATOM | 30 | N | LEU | A | 310 | 36.940 | -8.038 | 5.352 | 1.00 52.69 |
| | ATOM | 31 | CA | LEU | A | 310 | 36.877 | -6.759 | 4.658 | 1.00 48.20 |
| | ATOM | 32 | CB | LEU | A | 310 | 35.516 | -6.596 | 3.974 | 1.00 48.32 |
| 50 | ATOM | 33 | CG | LEU | A | 310 | 35.301 | -7.188 | 2.583 | 1.00 44.94 |
| | ATOM | 34 | CD1 | LEU | A | 310 | 33.951 | -6.728 | 2.055 | 1.00 46.45 |
| | ATOM | 35 | CD2 | LEU | A | 310 | 36.417 | -6.755 | 1.650 | 1.00 43.19 |
| | ATOM | 36 | C | LEU | A | 310 | 37.086 | -5.589 | 5.609 | 1.00 46.44 |
| | ATOM | 37 | O | LEU | A | 310 | 36.605 | -5.607 | 6.741 | 1.00 46.78 |
| 55 | ATOM | 38 | N | THR | A | 311 | 37.812 | -4.576 | 5.148 | 1.00 44.36 |
| | ATOM | 39 | CA | THR | A | 311 | 38.034 | -3.380 | 5.949 | 1.00 42.88 |
| | ATOM | 40 | CB | THR | A | 311 | 39.313 | -2.633 | 5.532 | 1.00 42.31 |
| | ATOM | 41 | OG1 | THR | A | 311 | 39.079 | -1.936 | 4.303 | 1.00 42.50 |
| | ATOM | 42 | CG2 | THR | A | 311 | 40.464 | -3.606 | 5.350 | 1.00 46.02 |
| 60 | ATOM | 43 | C | THR | A | 311 | 36.834 | -2.475 | 5.674 | 1.00 43.21 |

| | | | | | | | | | | | |
|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 44 | O | THR | A | 311 | 36.021 | -2.776 | 4.800 | 1.00 | 42.12 |
| | ATOM | 45 | N | ALA | A | 312 | 36.726 | -1.372 | 6.409 | 1.00 | 42.16 |
| | ATOM | 46 | CA | ALA | A | 312 | 35.616 | -0.444 | 6.228 | 1.00 | 40.10 |
| | ATOM | 47 | CB | ALA | A | 312 | 35.741 | 0.709 | 7.205 | 1.00 | 40.07 |
| | ATOM | 48 | C | ALA | A | 312 | 35.561 | 0.090 | 4.799 | 1.00 | 41.80 |
| 10 | ATOM | 49 | O | ALA | A | 312 | 34.510 | 0.074 | 4.154 | 1.00 | 37.81 |
| | ATOM | 50 | N | ASP | A | 313 | 36.698 | 0.564 | 4.304 | 1.00 | 42.35 |
| | ATOM | 51 | CA | ASP | A | 313 | 36.752 | 1.104 | 2.953 | 1.00 | 42.27 |
| | ATOM | 52 | CB | ASP | A | 313 | 38.133 | 1.703 | 2.680 | 1.00 | 43.74 |
| | ATOM | 53 | CG | ASP | A | 313 | 38.323 | 3.054 | 3.348 | 1.00 | 46.62 |
| 15 | ATOM | 54 | OD1 | ASP | A | 313 | 39.414 | 3.645 | 3.205 | 1.00 | 51.01 |
| | ATOM | 55 | OD2 | ASP | A | 313 | 37.380 | 3.529 | 4.015 | 1.00 | 48.89 |
| | ATOM | 56 | C | ASP | A | 313 | 36.422 | 0.027 | 1.926 | 1.00 | 38.68 |
| | ATOM | 57 | O | ASP | A | 313 | 35.704 | 0.281 | 0.959 | 1.00 | 38.75 |
| | ATOM | 58 | N | GLN | A | 314 | 36.931 | -1.179 | 2.145 | 1.00 | 34.76 |
| 20 | ATOM | 59 | CA | GLN | A | 314 | 36.666 | -2.277 | 1.229 | 1.00 | 33.55 |
| | ATOM | 60 | CB | GLN | A | 314 | 37.462 | -3.512 | 1.643 | 1.00 | 36.90 |
| | ATOM | 61 | CG | GLN | A | 314 | 38.963 | -3.384 | 1.436 | 1.00 | 40.45 |
| | ATOM | 62 | CD | GLN | A | 314 | 39.700 | -4.610 | 1.905 | 1.00 | 43.13 |
| | ATOM | 63 | OE1 | GLN | A | 314 | 39.394 | -5.196 | 2.935 | 1.00 | 43.60 |
| 25 | ATOM | 64 | NE2 | GLN | A | 314 | 40.701 | -5.032 | 1.117 | 1.00 | 44.03 |
| | ATOM | 65 | C | GLN | A | 314 | 35.176 | -2.595 | 1.201 | 1.00 | 34.95 |
| | ATOM | 66 | O | GLN | A | 314 | 34.605 | -2.860 | 0.140 | 1.00 | 32.89 |
| | ATOM | 67 | N | MET | A | 315 | 34.542 | -2.564 | 2.374 | 1.00 | 32.54 |
| | ATOM | 68 | CA | MET | A | 315 | 33.115 | -2.848 | 2.470 | 1.00 | 35.46 |
| 30 | ATOM | 69 | CB | MET | A | 315 | 32.650 | -2.794 | 3.926 | 1.00 | 37.09 |
| | ATOM | 70 | CG | MET | A | 315 | 31.137 | -2.777 | 4.097 | 1.00 | 39.42 |
| | ATOM | 71 | SD | MET | A | 315 | 30.443 | -4.426 | 4.053 | 1.00 | 46.55 |
| | ATOM | 72 | CE | MET | A | 315 | 31.351 | -5.205 | 5.397 | 1.00 | 45.29 |
| | ATOM | 73 | C | MET | A | 315 | 32.311 | -1.859 | 1.640 | 1.00 | 31.83 |
| 35 | ATOM | 74 | O | MET | A | 315 | 31.453 | -2.247 | 0.852 | 1.00 | 32.10 |
| | ATOM | 75 | N | VAL | A | 316 | 32.587 | -0.560 | 1.830 | 1.00 | 32.62 |
| | ATOM | 76 | CA | VAL | A | 316 | 31.882 | 0.470 | 1.079 | 1.00 | 31.09 |
| | ATOM | 77 | CB | VAL | A | 316 | 32.395 | 1.888 | 1.425 | 1.00 | 34.77 |
| | ATOM | 78 | CG1 | VAL | A | 316 | 31.786 | 2.899 | 0.461 | 1.00 | 34.10 |
| 40 | ATOM | 79 | CG2 | VAL | A | 316 | 32.021 | 2.246 | 2.862 | 1.00 | 34.40 |
| | ATOM | 80 | C | VAL | A | 316 | 32.092 | 0.232 | -0.414 | 1.00 | 33.48 |
| | ATOM | 81 | O | VAL | A | 316 | 31.145 | 0.266 | -1.200 | 1.00 | 32.49 |
| | ATOM | 82 | N | SER | A | 317 | 33.337 | -0.027 | -0.795 | 1.00 | 33.49 |
| | ATOM | 83 | CA | SER | A | 317 | 33.682 | -0.280 | -2.187 | 1.00 | 32.88 |
| 45 | ATOM | 84 | CB | SER | A | 317 | 35.165 | -0.635 | -2.297 | 1.00 | 35.77 |
| | ATOM | 85 | OG | SER | A | 317 | 35.825 | 0.277 | -3.154 | 1.00 | 42.70 |
| | ATOM | 86 | C | SER | A | 317 | 32.849 | -1.396 | -2.801 | 1.00 | 30.71 |
| | ATOM | 87 | O | SER | A | 317 | 32.279 | -1.238 | -3.880 | 1.00 | 31.14 |
| | ATOM | 88 | N | ALA | A | 318 | 32.792 | -2.529 | -2.111 | 1.00 | 29.51 |
| 50 | ATOM | 89 | CA | ALA | A | 318 | 32.035 | -3.676 | -2.580 | 1.00 | 29.93 |
| | ATOM | 90 | CB | ALA | A | 318 | 32.156 | -4.811 | -1.579 | 1.00 | 28.56 |
| | ATOM | 91 | C | ALA | A | 318 | 30.565 | -3.305 | -2.771 | 1.00 | 31.55 |
| | ATOM | 92 | O | ALA | A | 318 | 29.961 | -3.642 | -3.784 | 1.00 | 30.64 |
| | ATOM | 93 | N | LEU | A | 319 | 29.997 | -2.614 | -1.791 | 1.00 | 34.13 |
| 55 | ATOM | 94 | CA | LEU | A | 319 | 28.597 | -2.212 | -1.861 | 1.00 | 32.93 |
| | ATOM | 95 | CB | LEU | A | 319 | 28.170 | -1.576 | -0.540 | 1.00 | 31.15 |
| | ATOM | 96 | CG | LEU | A | 319 | 28.076 | -2.555 | 0.632 | 1.00 | 32.27 |
| | ATOM | 97 | CD1 | LEU | A | 319 | 27.523 | -1.840 | 1.852 | 1.00 | 32.14 |
| | ATOM | 98 | CD2 | LEU | A | 319 | 27.194 | -3.733 | 0.243 | 1.00 | 31.82 |
| 60 | ATOM | 99 | C | LEU | A | 319 | 28.340 | -1.257 | -3.020 | 1.00 | 34.41 |
| | ATOM | 100 | O | LEU | A | 319 | 27.430 | -1.475 | -3.818 | 1.00 | 35.23 |

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|----|------|-----|-----|------|---|-----|--------|--------|---------|------|-------|
| 5 | ATOM | 101 | N | LEU | A | 320 | 29.140 | -0.195 | -3.120 | 1.00 | 32.53 |
| | ATOM | 102 | CA | LEU | A | 320 | 28.972 | 0.756 | -4.212 | 1.00 | 35.33 |
| | ATOM | 103 | CB | LEU | A | 320 | 30.052 | 1.839 | -4.155 | 1.00 | 33.52 |
| | ATOM | 104 | CG | LEU | A | 320 | 29.974 | 2.899 | -3.054 | 1.00 | 34.60 |
| | ATOM | 105 | CD1 | LEU | A | 320 | 31.060 | 3.940 | -3.292 | 1.00 | 33.69 |
| 10 | ATOM | 106 | CD2 | LEU | A | 320 | 28.611 | 3.562 | -3.044 | 1.00 | 31.05 |
| | ATOM | 107 | C | LEU | A | 320 | 29.052 | 0.040 | -5.561 | 1.00 | 35.41 |
| | ATOM | 108 | O | LEU | A | 320 | 28.230 | 0.271 | -6.446 | 1.00 | 39.16 |
| | ATOM | 109 | N | AASP | A | 321 | 30.042 | -0.833 | -5.720 | 0.50 | 36.33 |
| | ATOM | 110 | N | BASP | A | 321 | 30.041 | -0.839 | -5.695 | 0.50 | 35.76 |
| 15 | ATOM | 111 | CA | AASP | A | 321 | 30.214 | -1.559 | -6.977 | 0.50 | 37.71 |
| | ATOM | 112 | CA | BASP | A | 321 | 30.258 | -1.595 | -6.925 | 0.50 | 37.11 |
| | ATOM | 113 | CB | AASP | A | 321 | 31.537 | -2.334 | -6.973 | 0.50 | 40.01 |
| | ATOM | 114 | CB | BASP | A | 321 | 31.573 | -2.374 | -6.826 | 0.50 | 39.41 |
| | ATOM | 115 | CG | AASP | A | 321 | 31.694 | -3.230 | -8.195 | 0.50 | 41.93 |
| 20 | ATOM | 116 | CG | BASP | A | 321 | 32.770 | -1.562 | -7.284 | 0.50 | 39.96 |
| | ATOM | 117 | OD1 | AASP | A | 321 | 31.523 | -2.733 | -9.329 | 0.50 | 42.11 |
| | ATOM | 118 | OD1 | BASP | A | 321 | 33.312 | -1.868 | -8.366 | 0.50 | 43.41 |
| | ATOM | 119 | OD2 | AASP | A | 321 | 31.988 | -4.432 | -8.022 | 0.50 | 42.69 |
| | ATOM | 120 | OD2 | BASP | A | 321 | 33.170 | -0.622 | -6.564 | 0.50 | 41.33 |
| 25 | ATOM | 121 | C | AASP | A | 321 | 29.069 | -2.524 | -7.275 | 0.50 | 37.19 |
| | ATOM | 122 | C | BASP | A | 321 | 29.123 | -2.565 | -7.253 | 0.50 | 36.68 |
| | ATOM | 123 | O | AASP | A | 321 | 28.820 | -2.861 | -8.434 | 0.50 | 36.87 |
| | ATOM | 124 | O | BASP | A | 321 | 28.934 | -2.942 | -8.411 | 0.50 | 36.08 |
| | ATOM | 125 | N | ALA | A | 322 | 28.374 | -2.968 | -6.235 | 1.00 | 35.35 |
| 30 | ATOM | 126 | CA | ALA | A | 322 | 27.268 | -3.902 | -6.417 | 1.00 | 31.59 |
| | ATOM | 127 | CB | ALA | A | 322 | 27.124 | -4.781 | -5.175 | 1.00 | 30.73 |
| | ATOM | 128 | C | ALA | A | 322 | 25.946 | -3.204 | -6.709 | 1.00 | 30.07 |
| | ATOM | 129 | O | ALA | A | 322 | 24.955 | -3.857 | -7.036 | 1.00 | 26.53 |
| | ATOM | 130 | N | GLU | A | 323 | 25.932 | -1.880 | -6.596 | 1.00 | 27.98 |
| 35 | ATOM | 131 | CA | GLU | A | 323 | 24.713 | -1.117 | -6.827 | 1.00 | 29.88 |
| | ATOM | 132 | CB | GLU | A | 323 | 25.027 | 0.380 | -6.855 | 1.00 | 30.98 |
| | ATOM | 133 | CG | GLU | A | 323 | 24.870 | 1.068 | -5.509 | 1.00 | 31.62 |
| | ATOM | 134 | CD | GLU | A | 323 | 23.463 | 0.940 | -4.960 | 1.00 | 31.98 |
| | ATOM | 135 | OE1 | GLU | A | 323 | 23.183 | -0.056 | -4.257 | 1.00 | 33.10 |
| 40 | ATOM | 136 | OE2 | GLU | A | 323 | 22.640 | 1.836 | -5.233 | 1.00 | 30.01 |
| | ATOM | 137 | C | GLU | A | 323 | 24.010 | -1.515 | -8.123 | 1.00 | 30.86 |
| | ATOM | 138 | O | GLU | A | 323 | 24.655 | -1.705 | -9.151 | 1.00 | 28.86 |
| | ATOM | 139 | N | PRO | A | 324 | 22.674 | -1.659 | -8.083 | 1.00 | 30.66 |
| | ATOM | 140 | CD | PRO | A | 324 | 21.774 | -1.466 | -6.935 | 1.00 | 31.01 |
| 45 | ATOM | 141 | CA | PRO | A | 324 | 21.935 | -2.032 | -9.290 | 1.00 | 30.29 |
| | ATOM | 142 | CB | PRO | A | 324 | 20.613 | -2.598 | -8.760 | 1.00 | 31.42 |
| | ATOM | 143 | CG | PRO | A | 324 | 20.626 | -2.363 | -7.258 | 1.00 | 33.66 |
| | ATOM | 144 | C | PRO | A | 324 | 21.717 | -0.785 | -10.138 | 1.00 | 27.46 |
| | ATOM | 145 | O | PRO | A | 324 | 21.893 | 0.332 | -9.668 | 1.00 | 26.19 |
| 50 | ATOM | 146 | N | PRO | A | 325 | 21.335 | -0.959 | -11.403 | 1.00 | 27.80 |
| | ATOM | 147 | CD | PRO | A | 325 | 21.082 | -2.198 | -12.161 | 1.00 | 27.35 |
| | ATOM | 148 | CA | PRO | A | 325 | 21.125 | 0.242 | -12.211 | 1.00 | 25.59 |
| | ATOM | 149 | CB | PRO | A | 325 | 21.258 | -0.266 | -13.637 | 1.00 | 24.02 |
| | ATOM | 150 | CG | PRO | A | 325 | 20.773 | -1.695 | -13.559 | 1.00 | 26.00 |
| 55 | ATOM | 151 | C | PRO | A | 325 | 19.749 | 0.830 | -11.954 | 1.00 | 23.73 |
| | ATOM | 152 | O | PRO | A | 325 | 18.873 | 0.165 | -11.402 | 1.00 | 24.83 |
| | ATOM | 153 | N | ILE | A | 326 | 19.571 | 2.081 | -12.352 | 1.00 | 22.11 |
| | ATOM | 154 | CA | ILE | A | 326 | 18.296 | 2.762 | -12.212 | 1.00 | 24.01 |
| | ATOM | 155 | CB | ILE | A | 326 | 18.502 | 4.282 | -12.133 | 1.00 | 25.97 |
| 60 | ATOM | 156 | CG2 | ILE | A | 326 | 17.168 | 4.992 | -12.286 | 1.00 | 20.75 |
| | ATOM | 157 | CG1 | ILE | A | 326 | 19.189 | 4.632 | -10.805 | 1.00 | 29.31 |

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|----|------|-----|-----|-----|---|-----|--------|---------------|------|-------|
| 5 | ATOM | 158 | CD1 | ILE | A | 326 | 19.301 | 6.120-10.525 | 1.00 | 32.91 |
| | ATOM | 159 | C | ILE | A | 326 | 17.506 | 2.408-13.471 | 1.00 | 25.72 |
| | ATOM | 160 | O | ILE | A | 326 | 17.906 | 2.758-14.581 | 1.00 | 25.55 |
| | ATOM | 161 | N | LEU | A | 327 | 16.392 | 1.703-13.301 | 1.00 | 25.57 |
| | ATOM | 162 | CA | LEU | A | 327 | 15.595 | 1.279-14.439 | 1.00 | 23.80 |
| 10 | ATOM | 163 | CB | LEU | A | 327 | 14.872 | -0.029-14.104 | 1.00 | 23.96 |
| | ATOM | 164 | CG | LEU | A | 327 | 15.778 | -1.210-13.728 | 1.00 | 19.89 |
| | ATOM | 165 | CD1 | LEU | A | 327 | 14.944 | -2.462-13.583 | 1.00 | 21.19 |
| | ATOM | 166 | CD2 | LEU | A | 327 | 16.850 | -1.415-14.805 | 1.00 | 17.53 |
| | ATOM | 167 | C | LEU | A | 327 | 14.598 | 2.317-14.935 | 1.00 | 27.16 |
| 15 | ATOM | 168 | O | LEU | A | 327 | 14.161 | 3.202-14.194 | 1.00 | 25.98 |
| | ATOM | 169 | N | TYR | A | 328 | 14.251 | 2.207-16.210 | 1.00 | 26.56 |
| | ATOM | 170 | CA | TYR | A | 328 | 13.303 | 3.123-16.814 | 1.00 | 24.45 |
| | ATOM | 171 | CB | TYR | A | 328 | 13.724 | 3.465-18.245 | 1.00 | 26.72 |
| | ATOM | 172 | CG | TYR | A | 328 | 14.587 | 4.693-18.314 | 1.00 | 27.73 |
| 20 | ATOM | 173 | CD1 | TYR | A | 328 | 14.021 | 5.949-18.518 | 1.00 | 28.56 |
| | ATOM | 174 | CE1 | TYR | A | 328 | 14.798 | 7.092-18.509 | 1.00 | 29.10 |
| | ATOM | 175 | CD2 | TYR | A | 328 | 15.962 | 4.612-18.110 | 1.00 | 26.01 |
| | ATOM | 176 | CE2 | TYR | A | 328 | 16.750 | 5.753-18.098 | 1.00 | 30.63 |
| | ATOM | 177 | CZ | TYR | A | 328 | 16.157 | 6.988-18.297 | 1.00 | 30.07 |
| 25 | ATOM | 178 | OH | TYR | A | 328 | 16.917 | 8.130-18.265 | 1.00 | 37.94 |
| | ATOM | 179 | C | TYR | A | 328 | 11.923 | 2.501-16.827 | 1.00 | 24.95 |
| | ATOM | 180 | O | TYR | A | 328 | 11.774 | 1.274-16.846 | 1.00 | 27.02 |
| | ATOM | 181 | N | SER | A | 329 | 10.912 | 3.358-16.800 | 1.00 | 25.60 |
| | ATOM | 182 | CA | SER | A | 329 | 9.533 | 2.908-16.837 | 1.00 | 29.45 |
| 30 | ATOM | 183 | CB | SER | A | 329 | 8.661 | 3.858-16.020 | 1.00 | 30.80 |
| | ATOM | 184 | OG | SER | A | 329 | 7.297 | 3.721-16.364 | 1.00 | 33.74 |
| | ATOM | 185 | C | SER | A | 329 | 9.129 | 2.947-18.313 | 1.00 | 31.30 |
| | ATOM | 186 | O | SER | A | 329 | 9.908 | 3.397-19.154 | 1.00 | 27.35 |
| | ATOM | 187 | N | GLU | A | 330 | 7.930 | 2.469-18.629 | 1.00 | 32.98 |
| 35 | ATOM | 188 | CA | GLU | A | 330 | 7.459 | 2.482-20.007 | 1.00 | 35.10 |
| | ATOM | 189 | CB | GLU | A | 330 | 6.031 | 1.968-20.074 | 1.00 | 34.67 |
| | ATOM | 190 | C | GLU | A | 330 | 7.532 | 3.924-20.505 | 1.00 | 40.06 |
| | ATOM | 191 | O | GLU | A | 330 | 7.068 | 4.841-19.826 | 1.00 | 42.65 |
| | ATOM | 192 | N | TYR | A | 331 | 8.124 | 4.126-21.681 | 1.00 | 41.16 |
| 40 | ATOM | 193 | CA | TYR | A | 331 | 8.263 | 5.470-22.234 | 1.00 | 42.66 |
| | ATOM | 194 | CB | TYR | A | 331 | 9.323 | 5.482-23.350 | 1.00 | 42.54 |
| | ATOM | 195 | CG | TYR | A | 331 | 9.202 | 4.347-24.345 | 1.00 | 38.67 |
| | ATOM | 196 | CD1 | TYR | A | 331 | 10.105 | 3.284-24.334 | 1.00 | 34.66 |
| | ATOM | 197 | CE1 | TYR | A | 331 | 9.985 | 2.228-25.233 | 1.00 | 34.89 |
| 45 | ATOM | 198 | CD2 | TYR | A | 331 | 8.174 | 4.327-25.287 | 1.00 | 37.88 |
| | ATOM | 199 | CE2 | TYR | A | 331 | 8.045 | 3.276-26.193 | 1.00 | 34.65 |
| | ATOM | 200 | CZ | TYR | A | 331 | 8.950 | 2.232-26.159 | 1.00 | 30.73 |
| | ATOM | 201 | OH | TYR | A | 331 | 8.814 | 1.191-27.042 | 1.00 | 30.97 |
| | ATOM | 202 | C | TYR | A | 331 | 6.943 | 6.043-22.754 | 1.00 | 46.24 |
| 50 | ATOM | 203 | O | TYR | A | 331 | 6.018 | 5.301-23.096 | 1.00 | 45.38 |
| | ATOM | 204 | N | ASP | A | 332 | 6.868 | 7.372-22.792 | 1.00 | 49.11 |
| | ATOM | 205 | CA | ASP | A | 332 | 5.684 | 8.092-23.262 | 1.00 | 52.40 |
| | ATOM | 206 | CB | ASP | A | 332 | 5.781 | 8.321-24.772 | 1.00 | 52.86 |
| | ATOM | 207 | C | ASP | A | 332 | 4.356 | 7.410-22.926 | 1.00 | 52.90 |
| 55 | ATOM | 208 | O | ASP | A | 332 | 3.561 | 7.116-23.818 | 1.00 | 53.94 |
| | ATOM | 209 | N | PRO | A | 333 | 4.103 | 7.144-21.632 | 1.00 | 53.63 |
| | ATOM | 210 | CD | PRO | A | 333 | 4.962 | 7.418-20.465 | 1.00 | 53.63 |
| | ATOM | 211 | CA | PRO | A | 333 | 2.840 | 6.497-21.253 | 1.00 | 53.55 |
| | ATOM | 212 | CB | PRO | A | 333 | 3.070 | 6.076-19.802 | 1.00 | 53.78 |
| 60 | ATOM | 213 | CG | PRO | A | 333 | 4.101 | 7.028-19.290 | 1.00 | 53.42 |
| | ATOM | 214 | C | PRO | A | 333 | 1.673 | 7.478-21.398 | 1.00 | 52.17 |

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|----|------|-----|-----|-----|---|-----|--------|---------------|------|-------|
| 5 | ATOM | 215 | O | PRO | A | 333 | 1.879 | 8.690-21.395 | 1.00 | 51.19 |
| | ATOM | 216 | N | THR | A | 334 | 0.457 | 6.956-21.532 | 1.00 | 52.26 |
| | ATOM | 217 | CA | THR | A | 334 | -0.724 | 7.802-21.687 | 1.00 | 54.21 |
| | ATOM | 218 | CB | THR | A | 334 | -1.997 | 6.949-21.813 | 1.00 | 53.90 |
| | ATOM | 219 | OG1 | THR | A | 334 | -1.971 | 6.256-23.065 | 1.00 | 53.92 |
| 10 | ATOM | 220 | CG2 | THR | A | 334 | -3.237 | 7.821-21.761 | 1.00 | 54.15 |
| | ATOM | 221 | C | THR | A | 334 | -0.864 | 8.782-20.525 | 1.00 | 56.34 |
| | ATOM | 222 | O | THR | A | 334 | -1.389 | 8.443-19.461 | 1.00 | 56.44 |
| | ATOM | 223 | N | ARG | A | 335 | -0.386 | 10.002-20.766 | 1.00 | 58.24 |
| | ATOM | 224 | CA | ARG | A | 335 | -0.377 | 11.099-19.801 | 1.00 | 57.96 |
| 15 | ATOM | 225 | CB | ARG | A | 335 | -0.569 | 12.427-20.531 | 1.00 | 60.22 |
| | ATOM | 226 | C | ARG | A | 335 | -1.349 | 10.996-18.627 | 1.00 | 56.61 |
| | ATOM | 227 | O | ARG | A | 335 | -0.919 | 10.908-17.475 | 1.00 | 60.70 |
| | ATOM | 228 | N | PRO | A | 336 | -2.667 | 11.015-18.889 | 1.00 | 52.43 |
| | ATOM | 229 | CD | PRO | A | 336 | -3.389 | 11.117-20.165 | 1.00 | 49.06 |
| 20 | ATOM | 230 | CA | PRO | A | 336 | -3.587 | 10.915-17.752 | 1.00 | 49.58 |
| | ATOM | 231 | CB | PRO | A | 336 | -4.911 | 11.456-18.302 | 1.00 | 48.66 |
| | ATOM | 232 | CG | PRO | A | 336 | -4.645 | 11.809-19.760 | 1.00 | 51.33 |
| | ATOM | 233 | C | PRO | A | 336 | -3.698 | 9.468-17.279 | 1.00 | 49.25 |
| | ATOM | 234 | O | PRO | A | 336 | -4.340 | 8.644-17.929 | 1.00 | 48.06 |
| 25 | ATOM | 235 | N | PHE | A | 337 | -3.063 | 9.170-16.147 | 1.00 | 47.90 |
| | ATOM | 236 | CA | PHE | A | 337 | -3.055 | 7.821-15.582 | 1.00 | 46.61 |
| | ATOM | 237 | CB | PHE | A | 337 | -2.063 | 7.732-14.421 | 1.00 | 47.73 |
| | ATOM | 238 | CG | PHE | A | 337 | -0.649 | 8.011-14.805 | 1.00 | 46.27 |
| | ATOM | 239 | CD1 | PHE | A | 337 | -0.017 | 9.168-14.368 | 1.00 | 46.55 |
| 30 | ATOM | 240 | CD2 | PHE | A | 337 | 0.061 | 7.113-15.591 | 1.00 | 48.12 |
| | ATOM | 241 | CE1 | PHE | A | 337 | 1.305 | 9.429-14.707 | 1.00 | 48.09 |
| | ATOM | 242 | CE2 | PHE | A | 337 | 1.386 | 7.364-15.938 | 1.00 | 47.57 |
| | ATOM | 243 | CZ | PHE | A | 337 | 2.009 | 8.525-15.495 | 1.00 | 48.40 |
| | ATOM | 244 | C | PHE | A | 337 | -4.401 | 7.338-15.071 | 1.00 | 46.15 |
| 35 | ATOM | 245 | O | PHE | A | 337 | -5.250 | 8.127-14.671 | 1.00 | 48.34 |
| | ATOM | 246 | N | SER | A | 338 | -4.573 | 6.022-15.080 | 1.00 | 45.06 |
| | ATOM | 247 | CA | SER | A | 338 | -5.781 | 5.385-14.578 | 1.00 | 45.12 |
| | ATOM | 248 | CB | SER | A | 338 | -6.477 | 4.594-15.684 | 1.00 | 44.49 |
| | ATOM | 249 | OG | SER | A | 338 | -6.227 | 3.206-15.554 | 1.00 | 45.78 |
| 40 | ATOM | 250 | C | SER | A | 338 | -5.292 | 4.439-13.488 | 1.00 | 47.04 |
| | ATOM | 251 | O | SER | A | 338 | -4.090 | 4.186-13.387 | 1.00 | 44.08 |
| | ATOM | 252 | N | GLU | A | 339 | -6.206 | 3.916-12.676 | 1.00 | 45.63 |
| | ATOM | 253 | CA | GLU | A | 339 | -5.802 | 3.012-11.608 | 1.00 | 45.40 |
| 45 | ATOM | 254 | CB | GLU | A | 339 | -7.015 | 2.521-10.814 | 1.00 | 45.66 |
| | ATOM | 255 | CG | GLU | A | 339 | -6.637 | 1.680 -9.600 | 1.00 | 46.81 |
| | ATOM | 256 | CD | GLU | A | 339 | -7.717 | 1.652 -8.535 | 1.00 | 47.56 |
| | ATOM | 257 | OE1 | GLU | A | 339 | -8.471 | 0.656 -8.477 | 1.00 | 47.37 |
| | ATOM | 258 | OE2 | GLU | A | 339 | -7.810 | 2.625 -7.754 | 1.00 | 49.29 |
| | ATOM | 259 | C | GLU | A | 339 | -5.040 | 1.821-12.170 | 1.00 | 45.23 |
| 50 | ATOM | 260 | O | GLU | A | 339 | -3.862 | 1.641-11.872 | 1.00 | 46.51 |
| | ATOM | 261 | N | ALA | A | 340 | -5.712 | 1.010-12.982 | 1.00 | 42.87 |
| | ATOM | 262 | CA | ALA | A | 340 | -5.078 | -0.158-13.574 | 1.00 | 40.24 |
| | ATOM | 263 | CB | ALA | A | 340 | -6.055 | -0.871-14.496 | 1.00 | 41.40 |
| | ATOM | 264 | C | ALA | A | 340 | -3.837 | 0.273-14.350 | 1.00 | 38.83 |
| 55 | ATOM | 265 | O | ALA | A | 340 | -2.909 | -0.515-14.543 | 1.00 | 35.58 |
| | ATOM | 266 | N | SER | A | 341 | -3.836 | 1.535-14.773 | 1.00 | 35.79 |
| | ATOM | 267 | CA | SER | A | 341 | -2.742 | 2.133-15.537 | 1.00 | 36.58 |
| | ATOM | 268 | CB | SER | A | 341 | -3.231 | 3.454-16.154 | 1.00 | 39.01 |
| | ATOM | 269 | OG | SER | A | 341 | -2.211 | 4.130-16.864 | 1.00 | 36.09 |
| 60 | ATOM | 270 | C | SER | A | 341 | -1.480 | 2.376-14.691 | 1.00 | 35.63 |
| | ATOM | 271 | O | SER | A | 341 | -0.389 | 1.913-15.038 | 1.00 | 33.20 |

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|----|------|-----|-----|-----|---|-----|--------|---------------|------|-------|
| 5 | ATOM | 272 | N | MET | A | 342 | -1.626 | 3.115-13.595 | 1.00 | 35.92 |
| | ATOM | 273 | CA | MET | A | 342 | -0.498 | 3.396-12.708 | 1.00 | 35.88 |
| | ATOM | 274 | CB | MET | A | 342 | -0.912 | 4.396-11.623 | 1.00 | 35.96 |
| | ATOM | 275 | CG | MET | A | 342 | 0.241 | 5.218-11.059 | 1.00 | 38.02 |
| | ATOM | 276 | SD | MET | A | 342 | -0.308 | 6.374 -9.780 | 1.00 | 44.73 |
| 10 | ATOM | 277 | CE | MET | A | 342 | 0.626 | 7.815-10.205 | 1.00 | 42.49 |
| | ATOM | 278 | C | MET | A | 342 | -0.011 | 2.100-12.059 | 1.00 | 34.17 |
| | ATOM | 279 | O | MET | A | 342 | 1.195 | 1.880-11.909 | 1.00 | 33.40 |
| | ATOM | 280 | N | MET | A | 343 | -0.957 | 1.243-11.687 | 1.00 | 29.95 |
| | ATOM | 281 | CA | MET | A | 343 | -0.640 | -0.034-11.062 | 1.00 | 31.96 |
| 15 | ATOM | 282 | CB | MET | A | 343 | -1.921 | -0.810-10.751 | 1.00 | 31.70 |
| | ATOM | 283 | CG | MET | A | 343 | -2.667 | -0.337 -9.502 | 1.00 | 37.13 |
| | ATOM | 284 | SD | MET | A | 343 | -1.749 | -0.507 -7.940 | 1.00 | 36.00 |
| | ATOM | 285 | CE | MET | A | 343 | -1.468 | -2.299 -7.886 | 1.00 | 32.14 |
| | ATOM | 286 | C | MET | A | 343 | 0.234 | -0.875-11.979 | 1.00 | 31.72 |
| 20 | ATOM | 287 | O | MET | A | 343 | 1.159 | -1.558-11.527 | 1.00 | 30.26 |
| | ATOM | 288 | N | GLY | A | 344 | -0.069 | -0.823-13.272 | 1.00 | 29.04 |
| | ATOM | 289 | CA | GLY | A | 344 | 0.688 | -1.591-14.242 | 1.00 | 24.94 |
| | ATOM | 290 | C | GLY | A | 344 | 2.104 | -1.085-14.396 | 1.00 | 26.01 |
| | ATOM | 291 | O | GLY | A | 344 | 3.046 | -1.873-14.463 | 1.00 | 28.72 |
| 25 | ATOM | 292 | N | LEU | A | 345 | 2.257 | 0.232-14.471 | 1.00 | 26.97 |
| | ATOM | 293 | CA | LEU | A | 345 | 3.576 | 0.839-14.608 | 1.00 | 31.15 |
| | ATOM | 294 | CB | LEU | A | 345 | 3.459 | 2.361-14.753 | 1.00 | 30.06 |
| | ATOM | 295 | CG | LEU | A | 345 | 2.765 | 2.924-15.995 | 1.00 | 33.50 |
| | ATOM | 296 | CD1 | LEU | A | 345 | 2.901 | 4.439-15.999 | 1.00 | 33.52 |
| 30 | ATOM | 297 | CD2 | LEU | A | 345 | 3.379 | 2.324-17.257 | 1.00 | 33.22 |
| | ATOM | 298 | C | LEU | A | 345 | 4.433 | 0.534-13.383 | 1.00 | 30.31 |
| | ATOM | 299 | O | LEU | A | 345 | 5.564 | 0.061-13.505 | 1.00 | 32.80 |
| | ATOM | 300 | N | LEU | A | 346 | 3.884 | 0.813-12.205 | 1.00 | 27.83 |
| | ATOM | 301 | CA | LEU | A | 346 | 4.595 | 0.596-10.947 | 1.00 | 26.19 |
| 35 | ATOM | 302 | CB | LEU | A | 346 | 3.729 | 1.063 -9.783 | 1.00 | 24.51 |
| | ATOM | 303 | CG | LEU | A | 346 | 3.483 | 2.569 -9.682 | 1.00 | 26.33 |
| | ATOM | 304 | CD1 | LEU | A | 346 | 2.623 | 2.844 -8.463 | 1.00 | 27.33 |
| | ATOM | 305 | CD2 | LEU | A | 346 | 4.809 | 3.317 -9.587 | 1.00 | 24.89 |
| | ATOM | 306 | C | LEU | A | 346 | 5.032 | -0.848-10.707 | 1.00 | 25.72 |
| 40 | ATOM | 307 | O | LEU | A | 346 | 6.181 | -1.102-10.345 | 1.00 | 29.86 |
| | ATOM | 308 | N | THR | A | 347 | 4.117 | -1.793-10.891 | 1.00 | 23.80 |
| | ATOM | 309 | CA | THR | A | 347 | 4.436 | -3.196-10.674 | 1.00 | 23.91 |
| | ATOM | 310 | CB | THR | A | 347 | 3.164 | -4.058-10.641 | 1.00 | 26.39 |
| | ATOM | 311 | OG1 | THR | A | 347 | 2.421 | -3.860-11.849 | 1.00 | 24.57 |
| 45 | ATOM | 312 | CG2 | THR | A | 347 | 2.301 | -3.682 -9.444 | 1.00 | 23.98 |
| | ATOM | 313 | C | THR | A | 347 | 5.366 | -3.734-11.756 | 1.00 | 26.17 |
| | ATOM | 314 | O | THR | A | 347 | 6.176 | -4.622-11.496 | 1.00 | 27.44 |
| | ATOM | 315 | N | ASN | A | 348 | 5.242 | -3.197-12.970 | 1.00 | 25.48 |
| | ATOM | 316 | CA | ASN | A | 348 | 6.092 | -3.617-14.082 | 1.00 | 23.77 |
| 50 | ATOM | 317 | CB | ASN | A | 348 | 5.657 | -2.926-15.385 | 1.00 | 24.59 |
| | ATOM | 318 | CG | ASN | A | 348 | 6.522 | -3.302-16.571 | 1.00 | 29.93 |
| | ATOM | 319 | OD1 | ASN | A | 348 | 7.616 | -2.799-16.771 | 1.00 | 24.81 |
| | ATOM | 320 | ND2 | ASN | A | 348 | 6.010 | -4.236-17.391 | 1.00 | 32.61 |
| | ATOM | 321 | C | ASN | A | 348 | 7.532 | -3.229-13.741 | 1.00 | 22.82 |
| 55 | ATOM | 322 | O | ASN | A | 348 | 8.453 | -4.027-13.870 | 1.00 | 18.83 |
| | ATOM | 323 | N | LEU | A | 349 | 7.711 | -1.993-13.288 | 1.00 | 22.58 |
| | ATOM | 324 | CA | LEU | A | 349 | 9.030 | -1.507-12.914 | 1.00 | 21.85 |
| | ATOM | 325 | CB | LEU | A | 349 | 8.929 | -0.028-12.536 | 1.00 | 22.00 |
| | ATOM | 326 | CG | LEU | A | 349 | 10.155 | 0.673-11.953 | 1.00 | 23.64 |
| 60 | ATOM | 327 | CD1 | LEU | A | 349 | 11.224 | 0.826-13.017 | 1.00 | 19.35 |
| | ATOM | 328 | CD2 | LEU | A | 349 | 9.726 | 2.040-11.415 | 1.00 | 21.97 |

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|----|------|-----|-----|-----|---|-----|--------|----------------|------|-------|
| 5 | ATOM | 329 | C | LEU | A | 349 | 9.564 | -2.335-11.734 | 1.00 | 22.94 |
| | ATOM | 330 | O | LEU | A | 349 | 10.724 | -2.749-11.717 | 1.00 | 23.97 |
| | ATOM | 331 | N | ALA | A | 350 | 8.705 | -2.591-10.756 | 1.00 | 21.67 |
| | ATOM | 332 | CA | ALA | A | 350 | 9.113 | -3.356 -9.586 | 1.00 | 21.83 |
| | ATOM | 333 | CB | ALA | A | 350 | 7.963 | -3.441 -8.593 | 1.00 | 18.95 |
| 10 | ATOM | 334 | C | ALA | A | 350 | 9.568 | -4.757 -9.985 | 1.00 | 21.90 |
| | ATOM | 335 | O | ALA | A | 350 | 10.625 | -5.221 -9.554 | 1.00 | 24.15 |
| | ATOM | 336 | N | ASP | A | 351 | 8.767 | -5.423-10.810 | 1.00 | 23.24 |
| | ATOM | 337 | CA | ASP | A | 351 | 9.093 | -6.772-11.259 | 1.00 | 25.87 |
| | ATOM | 338 | CB | ASP | A | 351 | 8.028 | -7.274-12.239 | 1.00 | 27.03 |
| 15 | ATOM | 339 | CG | ASP | A | 351 | 8.103 | -8.772-12.458 | 1.00 | 31.64 |
| | ATOM | 340 | OD1 | ASP | A | 351 | 8.217 | -9.196-13.628 | 1.00 | 35.06 |
| | ATOM | 341 | OD2 | ASP | A | 351 | 8.049 | -9.525-11.464 | 1.00 | 36.86 |
| | ATOM | 342 | C | ASP | A | 351 | 10.469 | -6.825-11.912 | 1.00 | 22.36 |
| | ATOM | 343 | O | ASP | A | 351 | 11.219 | -7.773-11.702 | 1.00 | 25.15 |
| 20 | ATOM | 344 | N | ARG | A | 352 | 10.810 | -5.808-12.697 | 1.00 | 23.58 |
| | ATOM | 345 | CA | ARG | A | 352 | 12.115 | -5.787-13.347 | 1.00 | 21.07 |
| | ATOM | 346 | CB | ARG | A | 352 | 12.120 | -4.785-14.507 | 1.00 | 21.02 |
| | ATOM | 347 | CG | ARG | A | 352 | 11.539 | -5.352-15.797 | 1.00 | 20.44 |
| | ATOM | 348 | CD | ARG | A | 352 | 11.554 | -4.319-16.915 | 1.00 | 20.43 |
| 25 | ATOM | 349 | NE | ARG | A | 352 | 10.592 | -3.245-16.687 | 1.00 | 19.85 |
| | ATOM | 350 | CZ | ARG | A | 352 | 10.910 | -1.954-16.641 | 1.00 | 19.69 |
| | ATOM | 351 | NH1 | ARG | A | 352 | 12.172 | -1.564-16.813 | 1.00 | 17.36 |
| | ATOM | 352 | NH2 | ARG | A | 352 | 9.962 | -1.049-16.441 | 1.00 | 21.88 |
| | ATOM | 353 | C | ARG | A | 352 | 13.223 | -5.442-12.350 | 1.00 | 22.11 |
| 30 | ATOM | 354 | O | ARG | A | 352 | 14.346 | -5.945-12.454 | 1.00 | 24.13 |
| | ATOM | 355 | N | GLU | A | 353 | 12.909 | -4.587-11.383 | 1.00 | 18.66 |
| | ATOM | 356 | CA | GLU | A | 353 | 13.888 | -4.206-10.376 | 1.00 | 19.08 |
| | ATOM | 357 | CB | GLU | A | 353 | 13.317 | -3.102 -9.483 | 1.00 | 21.62 |
| | ATOM | 358 | CG | GLU | A | 353 | 13.295 | -1.718-10.114 | 1.00 | 20.97 |
| 35 | ATOM | 359 | CD | GLU | A | 353 | 12.832 | -0.648 -9.129 | 1.00 | 23.84 |
| | ATOM | 360 | OE1 | GLU | A | 353 | 11.611 | -0.531 -8.926 | 1.00 | 24.76 |
| | ATOM | 361 | OE2 | GLU | A | 353 | 13.686 | 0.066 -8.557 | 1.00 | 24.95 |
| | ATOM | 362 | C | GLU | A | 353 | 14.246 | -5.423 -9.512 | 1.00 | 20.14 |
| | ATOM | 363 | O | GLU | A | 353 | 15.398 | -5.600 -9.104 | 1.00 | 19.40 |
| 40 | ATOM | 364 | N | LEU | A | 354 | 13.246 | -6.257 -9.235 | 1.00 | 19.54 |
| | ATOM | 365 | CA | LEU | A | 354 | 13.434 | -7.452 -8.415 | 1.00 | 21.77 |
| | ATOM | 366 | CB | LEU | A | 354 | 12.107 | -8.209 -8.270 | 1.00 | 23.09 |
| | ATOM | 367 | CG | LEU | A | 354 | 11.160 | -7.606 -7.223 | 1.00 | 25.00 |
| | ATOM | 368 | CD1 | LEU | A | 354 | 9.720 | -8.013 -7.510 | 1.00 | 23.49 |
| 45 | ATOM | 369 | CD2 | LEU | A | 354 | 11.584 | -8.069 -5.839 | 1.00 | 23.31 |
| | ATOM | 370 | C | LEU | A | 354 | 14.500 | -8.386 -8.981 | 1.00 | 23.21 |
| | ATOM | 371 | O | LEU | A | 354 | 15.255 | -9.007 -8.234 | 1.00 | 22.44 |
| | ATOM | 372 | N | VAL | A | 355 | 14.560 | -8.490-10.302 | 1.00 | 22.52 |
| | ATOM | 373 | CA | VAL | A | 355 | 15.551 | -9.343-10.935 | 1.00 | 21.66 |
| 50 | ATOM | 374 | CB | VAL | A | 355 | 15.353 | -9.365-12.466 | 1.00 | 24.35 |
| | ATOM | 375 | CG1 | VAL | A | 355 | 16.435 | -10.214-13.119 | 1.00 | 28.16 |
| | ATOM | 376 | CG2 | VAL | A | 355 | 13.957 | -9.886-12.798 | 1.00 | 21.59 |
| | ATOM | 377 | C | VAL | A | 355 | 16.944 | -8.811-10.606 | 1.00 | 23.74 |
| | ATOM | 378 | O | VAL | A | 355 | 17.857 | -9.581-10.291 | 1.00 | 23.51 |
| 55 | ATOM | 379 | N | HIS | A | 356 | 17.105 | -7.489-10.669 | 1.00 | 21.27 |
| | ATOM | 380 | CA | HIS | A | 356 | 18.392 | -6.861-10.369 | 1.00 | 21.31 |
| | ATOM | 381 | CB | HIS | A | 356 | 18.384 | -5.390-10.811 | 1.00 | 19.87 |
| | ATOM | 382 | CG | HIS | A | 356 | 18.494 | -5.205-12.295 | 1.00 | 21.77 |
| | ATOM | 383 | CD2 | HIS | A | 356 | 17.543 | -5.048-13.248 | 1.00 | 21.66 |
| 60 | ATOM | 384 | ND1 | HIS | A | 356 | 19.704 | -5.177-12.955 | 1.00 | 21.11 |
| | ATOM | 385 | CE1 | HIS | A | 356 | 19.496 | -5.011-14.249 | 1.00 | 24.96 |

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|----|------|-----|-----|------|---|-----|--------|---------|---------|------|-------|
| 5 | ATOM | 386 | NE2 | HIS | A | 356 | 18.192 | -4.931 | -14.455 | 1.00 | 18.37 |
| | ATOM | 387 | C | HIS | A | 356 | 18.702 | -6.947 | -8.875 | 1.00 | 21.41 |
| | ATOM | 388 | O | HIS | A | 356 | 19.864 | -7.111 | -8.465 | 1.00 | 21.88 |
| | ATOM | 389 | N | MET | A | 357 | 17.660 | -6.843 | -8.058 | 1.00 | 21.84 |
| | ATOM | 390 | CA | MET | A | 357 | 17.837 | -6.906 | -6.610 | 1.00 | 21.51 |
| 10 | ATOM | 391 | CB | MET | A | 357 | 16.503 | -6.668 | -5.898 | 1.00 | 17.60 |
| | ATOM | 392 | CG | MET | A | 357 | 16.629 | -6.579 | -4.369 | 1.00 | 19.36 |
| | ATOM | 393 | SD | MET | A | 357 | 15.051 | -6.755 | -3.531 | 1.00 | 23.64 |
| | ATOM | 394 | CE | MET | A | 357 | 14.189 | -5.332 | -4.163 | 1.00 | 23.13 |
| | ATOM | 395 | C | MET | A | 357 | 18.411 | -8.259 | -6.192 | 1.00 | 23.69 |
| 15 | ATOM | 396 | O | MET | A | 357 | 19.337 | -8.328 | -5.389 | 1.00 | 24.41 |
| | ATOM | 397 | N | ILE | A | 358 | 17.856 | -9.331 | -6.746 | 1.00 | 27.14 |
| | ATOM | 398 | CA | ILE | A | 358 | 18.314 | -10.672 | -6.425 | 1.00 | 28.79 |
| | ATOM | 399 | CB | ILE | A | 358 | 17.529 | -11.725 | -7.232 | 1.00 | 32.42 |
| | ATOM | 400 | CG2 | ILE | A | 358 | 18.267 | -13.064 | -7.220 | 1.00 | 32.77 |
| 20 | ATOM | 401 | CG1 | ILE | A | 358 | 16.125 | -11.880 | -6.644 | 1.00 | 31.94 |
| | ATOM | 402 | CD1 | ILE | A | 358 | 15.062 | -12.196 | -7.680 | 1.00 | 34.85 |
| | ATOM | 403 | C | ILE | A | 358 | 19.801 | -10.802 | -6.728 | 1.00 | 28.75 |
| | ATOM | 404 | O | ILE | A | 358 | 20.569 | -11.305 | -5.912 | 1.00 | 31.60 |
| | ATOM | 405 | N | ASN | A | 359 | 20.207 | -10.325 | -7.897 | 1.00 | 27.91 |
| 25 | ATOM | 406 | CA | ASN | A | 359 | 21.601 | -10.401 | -8.293 | 1.00 | 29.16 |
| | ATOM | 407 | CB | ASN | A | 359 | 21.721 | -10.172 | -9.801 | 1.00 | 31.88 |
| | ATOM | 408 | CG | ASN | A | 359 | 21.253 | -11.381 | -10.599 | 1.00 | 39.34 |
| | ATOM | 409 | OD1 | ASN | A | 359 | 21.916 | -12.422 | -10.612 | 1.00 | 41.27 |
| | ATOM | 410 | ND2 | ASN | A | 359 | 20.102 | -11.255 | -11.253 | 1.00 | 38.58 |
| 30 | ATOM | 411 | C | ASN | A | 359 | 22.476 | -9.436 | -7.510 | 1.00 | 30.75 |
| | ATOM | 412 | O | ASN | A | 359 | 23.686 | -9.629 | -7.412 | 1.00 | 33.35 |
| | ATOM | 413 | N | TRP | A | 360 | 21.872 | -8.400 | -6.940 | 1.00 | 30.07 |
| | ATOM | 414 | CA | TRP | A | 360 | 22.634 | -7.451 | -6.132 | 1.00 | 27.87 |
| | ATOM | 415 | CB | TRP | A | 360 | 21.849 | -6.150 | -5.948 | 1.00 | 24.80 |
| 35 | ATOM | 416 | CG | TRP | A | 360 | 22.196 | -5.392 | -4.691 | 1.00 | 23.04 |
| | ATOM | 417 | CD2 | TRP | A | 360 | 21.501 | -5.443 | -3.438 | 1.00 | 19.83 |
| | ATOM | 418 | CE2 | TRP | A | 360 | 22.147 | -4.543 | -2.564 | 1.00 | 22.31 |
| | ATOM | 419 | CE3 | TRP | A | 360 | 20.392 | -6.165 | -2.972 | 1.00 | 20.09 |
| | ATOM | 420 | CD1 | TRP | A | 360 | 23.212 | -4.488 | -4.529 | 1.00 | 18.99 |
| 40 | ATOM | 421 | NE1 | TRP | A | 360 | 23.187 | -3.974 | -3.255 | 1.00 | 21.17 |
| | ATOM | 422 | CZ2 | TRP | A | 360 | 21.721 | -4.340 | -1.243 | 1.00 | 20.43 |
| | ATOM | 423 | CZ3 | TRP | A | 360 | 19.968 | -5.965 | -1.661 | 1.00 | 20.12 |
| | ATOM | 424 | CH2 | TRP | A | 360 | 20.635 | -5.057 | -0.812 | 1.00 | 18.54 |
| | ATOM | 425 | C | TRP | A | 360 | 22.892 | -8.099 | -4.766 | 1.00 | 24.88 |
| 45 | ATOM | 426 | O | TRP | A | 360 | 23.978 | -7.980 | -4.198 | 1.00 | 25.00 |
| | ATOM | 427 | N | ALA | A | 361 | 21.879 | -8.789 | -4.252 | 1.00 | 24.08 |
| | ATOM | 428 | CA | ALA | A | 361 | 21.972 | -9.462 | -2.958 | 1.00 | 26.06 |
| | ATOM | 429 | CB | ALA | A | 361 | 20.676 | -10.203 | -2.672 | 1.00 | 20.27 |
| | ATOM | 430 | C | ALA | A | 361 | 23.161 | -10.433 | -2.897 | 1.00 | 28.44 |
| 50 | ATOM | 431 | O | ALA | A | 361 | 23.843 | -10.531 | -1.876 | 1.00 | 28.95 |
| | ATOM | 432 | N | LYS | A | 362 | 23.414 | -11.144 | -3.992 | 1.00 | 31.41 |
| | ATOM | 433 | CA | LYS | A | 362 | 24.530 | -12.097 | -4.047 | 1.00 | 33.33 |
| | ATOM | 434 | CB | LYS | A | 362 | 24.564 | -12.824 | -5.390 | 1.00 | 34.81 |
| | ATOM | 435 | CG | LYS | A | 362 | 23.319 | -13.608 | -5.756 | 1.00 | 36.27 |
| 55 | ATOM | 436 | CD | LYS | A | 362 | 23.458 | -14.178 | -7.167 | 1.00 | 38.30 |
| | ATOM | 437 | CE | LYS | A | 362 | 22.369 | -15.193 | -7.472 | 1.00 | 40.94 |
| | ATOM | 438 | NZ | LYS | A | 362 | 22.111 | -15.322 | -8.937 | 1.00 | 42.49 |
| | ATOM | 439 | C | LYS | A | 362 | 25.854 | -11.351 | -3.893 | 1.00 | 34.17 |
| | ATOM | 440 | O | LYS | A | 362 | 26.880 | -11.977 | -3.595 | 1.00 | 35.40 |
| 60 | ATOM | 441 | N | AARG | A | 363 | 25.826 | -10.059 | -4.095 | 0.50 | 34.23 |
| | ATOM | 442 | N | BARG | A | 363 | 25.826 | -10.059 | -4.095 | 0.50 | 34.03 |

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|----|------|-----|-----|------|---|-----|--------|---------|---------|------|-------|
| 5 | ATOM | 443 | CA | AARG | A | 363 | 27.035 | -9.254 | -3.987 | 0.50 | 33.25 |
| | ATOM | 444 | CA | BARG | A | 363 | 27.035 | -9.254 | -3.987 | 0.50 | 32.83 |
| | ATOM | 445 | CB | AARG | A | 363 | 27.031 | -8.153 | -5.044 | 0.50 | 34.67 |
| | ATOM | 446 | CB | BARG | A | 363 | 27.031 | -8.153 | -5.045 | 0.50 | 34.20 |
| | ATOM | 447 | CG | AARG | A | 363 | 26.933 | -8.654 | -6.478 | 0.50 | 36.32 |
| 10 | ATOM | 448 | CG | BARG | A | 363 | 26.930 | -8.654 | -6.480 | 0.50 | 35.56 |
| | ATOM | 449 | CD | AARG | A | 363 | 27.745 | -7.775 | -7.415 | 0.50 | 38.39 |
| | ATOM | 450 | CD | BARG | A | 363 | 27.752 | -7.781 | -7.414 | 0.50 | 37.18 |
| | ATOM | 451 | NE | AARG | A | 363 | 29.171 | -7.793 | -7.091 | 0.50 | 39.98 |
| | ATOM | 452 | NE | BARG | A | 363 | 27.195 | -7.725 | -8.762 | 0.50 | 37.39 |
| 15 | ATOM | 453 | CZ | AARG | A | 363 | 30.086 | -7.038 | -7.692 | 0.50 | 40.54 |
| | ATOM | 454 | CZ | BARG | A | 363 | 27.905 | -7.457 | -9.855 | 0.50 | 40.02 |
| | ATOM | 455 | NH1 | AARG | A | 363 | 29.735 | -6.218 | -8.675 | 0.50 | 38.13 |
| | ATOM | 456 | NH1 | BARG | A | 363 | 29.205 | -7.191 | -9.761 | 0.50 | 40.42 |
| | ATOM | 457 | NH2 | AARG | A | 363 | 31.358 | -7.123 | -7.326 | 0.50 | 43.19 |
| 20 | ATOM | 458 | NH2 | BARG | A | 363 | 27.311 | -7.436 | -11.041 | 0.50 | 38.91 |
| | ATOM | 459 | C | AARG | A | 363 | 27.207 | -8.630 | -2.610 | 0.50 | 33.28 |
| | ATOM | 460 | C | BARG | A | 363 | 27.207 | -8.630 | -2.610 | 0.50 | 32.81 |
| | ATOM | 461 | O | AARG | A | 363 | 28.223 | -7.992 | -2.344 | 0.50 | 34.18 |
| | ATOM | 462 | O | BARG | A | 363 | 28.223 | -7.992 | -2.345 | 0.50 | 33.43 |
| 25 | ATOM | 463 | N | VAL | A | 364 | 26.215 | -8.798 | -1.740 | 1.00 | 33.12 |
| | ATOM | 464 | CA | VAL | A | 364 | 26.288 | -8.240 | -0.389 | 1.00 | 33.63 |
| | ATOM | 465 | CB | VAL | A | 364 | 24.898 | -8.178 | 0.292 | 1.00 | 34.97 |
| | ATOM | 466 | CG1 | VAL | A | 364 | 25.036 | -7.608 | 1.700 | 1.00 | 35.44 |
| | ATOM | 467 | CG2 | VAL | A | 364 | 23.946 | -7.328 | -0.532 | 1.00 | 36.69 |
| 30 | ATOM | 468 | C | VAL | A | 364 | 27.184 | -9.157 | 0.428 | 1.00 | 34.27 |
| | ATOM | 469 | O | VAL | A | 364 | 26.878 | -10.341 | 0.603 | 1.00 | 34.95 |
| | ATOM | 470 | N | PRO | A | 365 | 28.306 | -8.626 | 0.935 | 1.00 | 36.08 |
| | ATOM | 471 | CD | PRO | A | 365 | 28.775 | -7.235 | 0.793 | 1.00 | 34.84 |
| | ATOM | 472 | CA | PRO | A | 365 | 29.231 | -9.442 | 1.733 | 1.00 | 37.82 |
| 35 | ATOM | 473 | CB | PRO | A | 365 | 30.110 | -8.408 | 2.430 | 1.00 | 34.31 |
| | ATOM | 474 | CG | PRO | A | 365 | 30.127 | -7.247 | 1.475 | 1.00 | 37.77 |
| | ATOM | 475 | C | PRO | A | 365 | 28.538 | -10.373 | 2.720 | 1.00 | 37.61 |
| | ATOM | 476 | O | PRO | A | 365 | 27.692 | -9.945 | 3.507 | 1.00 | 37.74 |
| | ATOM | 477 | N | GLY | A | 366 | 28.890 | -11.654 | 2.654 | 1.00 | 39.04 |
| 40 | ATOM | 478 | CA | GLY | A | 366 | 28.307 | -12.635 | 3.554 | 1.00 | 38.27 |
| | ATOM | 479 | C | GLY | A | 366 | 26.991 | -13.264 | 3.138 | 1.00 | 39.32 |
| | ATOM | 480 | O | GLY | A | 366 | 26.638 | -14.336 | 3.635 | 1.00 | 39.53 |
| | ATOM | 481 | N | PHE | A | 367 | 26.246 | -12.615 | 2.236 | 1.00 | 38.60 |
| | ATOM | 482 | CA | PHE | A | 367 | 24.960 | -13.148 | 1.783 | 1.00 | 36.36 |
| 45 | ATOM | 483 | CB | PHE | A | 367 | 24.281 | -12.178 | 0.808 | 1.00 | 32.10 |
| | ATOM | 484 | CG | PHE | A | 367 | 22.827 | -12.473 | 0.581 | 1.00 | 30.12 |
| | ATOM | 485 | CD1 | PHE | A | 367 | 22.401 | -13.083 | -0.596 | 1.00 | 28.95 |
| | ATOM | 486 | CD2 | PHE | A | 367 | 21.882 | -12.176 | 1.563 | 1.00 | 26.18 |
| | ATOM | 487 | CE1 | PHE | A | 367 | 21.050 | -13.400 | -0.792 | 1.00 | 29.42 |
| 50 | ATOM | 488 | CE2 | PHE | A | 367 | 20.535 | -12.491 | 1.373 | 1.00 | 27.60 |
| | ATOM | 489 | CZ | PHE | A | 367 | 20.118 | -13.103 | 0.196 | 1.00 | 26.81 |
| | ATOM | 490 | C | PHE | A | 367 | 25.072 | -14.519 | 1.117 | 1.00 | 36.82 |
| | ATOM | 491 | O | PHE | A | 367 | 24.244 | -15.398 | 1.359 | 1.00 | 36.55 |
| | ATOM | 492 | N | VAL | A | 368 | 26.088 | -14.694 | 0.276 | 1.00 | 38.28 |
| 55 | ATOM | 493 | CA | VAL | A | 368 | 26.289 | -15.965 | -0.420 | 1.00 | 42.34 |
| | ATOM | 494 | CB | VAL | A | 368 | 27.386 | -15.850 | -1.504 | 1.00 | 41.78 |
| | ATOM | 495 | CG1 | VAL | A | 368 | 26.972 | -14.831 | -2.550 | 1.00 | 44.60 |
| | ATOM | 496 | CG2 | VAL | A | 368 | 28.707 | -15.457 | -0.873 | 1.00 | 42.23 |
| | ATOM | 497 | C | VAL | A | 368 | 26.664 | -17.100 | 0.533 | 1.00 | 43.85 |
| 60 | ATOM | 498 | O | VAL | A | 368 | 26.469 | -18.274 | 0.216 | 1.00 | 44.85 |
| | ATOM | 499 | N | ASP | A | 369 | 27.199 | -16.750 | 1.699 | 1.00 | 44.93 |

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|----|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 500 | CA | ASP | A | 369 | 27.579 | -17.755 | 2.688 | 1.00 | 44.96 |
| | ATOM | 501 | CB | ASP | A | 369 | 28.336 | -17.106 | 3.849 | 1.00 | 43.76 |
| | ATOM | 502 | CG | ASP | A | 369 | 29.608 | -16.413 | 3.404 | 1.00 | 43.04 |
| | ATOM | 503 | OD1 | ASP | A | 369 | 30.121 | -15.570 | 4.167 | 1.00 | 44.32 |
| | ATOM | 504 | OD2 | ASP | A | 369 | 30.097 | -16.709 | 2.293 | 1.00 | 46.76 |
| 10 | ATOM | 505 | C | ASP | A | 369 | 26.340 | -18.465 | 3.228 | 1.00 | 45.89 |
| | ATOM | 506 | O | ASP | A | 369 | 26.360 | -19.671 | 3.475 | 1.00 | 48.61 |
| | ATOM | 507 | N | LEU | A | 370 | 25.261 | -17.714 | 3.407 | 1.00 | 43.59 |
| | ATOM | 508 | CA | LEU | A | 370 | 24.020 | -18.279 | 3.924 | 1.00 | 44.24 |
| | ATOM | 509 | CB | LEU | A | 370 | 22.980 | -17.173 | 4.110 | 1.00 | 41.42 |
| 15 | ATOM | 510 | CG | LEU | A | 370 | 23.404 | -16.015 | 5.014 | 1.00 | 41.45 |
| | ATOM | 511 | CD1 | LEU | A | 370 | 22.219 | -15.095 | 5.245 | 1.00 | 42.25 |
| | ATOM | 512 | CD2 | LEU | A | 370 | 23.931 | -16.552 | 6.332 | 1.00 | 38.35 |
| | ATOM | 513 | C | LEU | A | 370 | 23.449 | -19.360 | 3.013 | 1.00 | 44.03 |
| | ATOM | 514 | O | LEU | A | 370 | 23.773 | -19.423 | 1.829 | 1.00 | 43.63 |
| 20 | ATOM | 515 | N | THR | A | 371 | 22.593 | -20.206 | 3.575 | 1.00 | 44.29 |
| | ATOM | 516 | CA | THR | A | 371 | 21.968 | -21.272 | 2.806 | 1.00 | 44.84 |
| | ATOM | 517 | CB | THR | A | 371 | 21.293 | -22.302 | 3.730 | 1.00 | 45.65 |
| | ATOM | 518 | OG1 | THR | A | 371 | 20.262 | -21.663 | 4.495 | 1.00 | 46.43 |
| | ATOM | 519 | CG2 | THR | A | 371 | 22.314 | -22.903 | 4.677 | 1.00 | 46.48 |
| 25 | ATOM | 520 | C | THR | A | 371 | 20.923 | -20.684 | 1.864 | 1.00 | 44.93 |
| | ATOM | 521 | O | THR | A | 371 | 20.418 | -19.585 | 2.092 | 1.00 | 44.36 |
| | ATOM | 522 | N | LEU | A | 372 | 20.607 | -21.418 | 0.804 | 1.00 | 43.83 |
| | ATOM | 523 | CA | LEU | A | 372 | 19.624 | -20.971 | -0.166 | 1.00 | 44.62 |
| | ATOM | 524 | CB | LEU | A | 372 | 19.407 | -22.043 | -1.237 | 1.00 | 47.17 |
| 30 | ATOM | 525 | CG | LEU | A | 372 | 18.512 | -21.690 | -2.429 | 1.00 | 46.91 |
| | ATOM | 526 | CD1 | LEU | A | 372 | 19.005 | -20.417 | -3.098 | 1.00 | 48.73 |
| | ATOM | 527 | CD2 | LEU | A | 372 | 18.521 | -22.844 | -3.420 | 1.00 | 51.12 |
| | ATOM | 528 | C | LEU | A | 372 | 18.307 | -20.644 | 0.512 | 1.00 | 44.84 |
| | ATOM | 529 | O | LEU | A | 372 | 17.705 | -19.602 | 0.261 | 1.00 | 43.25 |
| 35 | ATOM | 530 | N | HIS | A | 373 | 17.849 | -21.558 | 1.382 | 1.00 | 43.14 |
| | ATOM | 531 | CA | HIS | A | 373 | 16.599 | -21.353 | 2.100 | 1.00 | 42.23 |
| | ATOM | 532 | CB | HIS | A | 373 | 16.318 | -22.525 | 3.062 | 1.00 | 45.38 |
| | ATOM | 533 | CG | HIS | A | 373 | 15.114 | -22.315 | 3.934 | 1.00 | 51.43 |
| | ATOM | 534 | CD2 | HIS | A | 373 | 13.808 | -22.621 | 3.743 | 1.00 | 54.99 |
| 40 | ATOM | 535 | ND1 | HIS | A | 373 | 15.187 | -21.716 | 5.174 | 1.00 | 54.26 |
| | ATOM | 536 | CE1 | HIS | A | 373 | 13.979 | -21.663 | 5.709 | 1.00 | 53.77 |
| | ATOM | 537 | NE2 | HIS | A | 373 | 13.124 | -22.206 | 4.861 | 1.00 | 55.27 |
| | ATOM | 538 | C | HIS | A | 373 | 16.665 | -20.047 | 2.885 | 1.00 | 39.78 |
| | ATOM | 539 | O | HIS | A | 373 | 15.677 | -19.324 | 2.971 | 1.00 | 37.71 |
| 45 | ATOM | 540 | N | ASP | A | 374 | 17.839 | -19.738 | 3.440 | 1.00 | 36.38 |
| | ATOM | 541 | CA | ASP | A | 374 | 18.020 | -18.516 | 4.219 | 1.00 | 37.21 |
| | ATOM | 542 | CB | ASP | A | 374 | 19.287 | -18.620 | 5.073 | 1.00 | 38.17 |
| | ATOM | 543 | CG | ASP | A | 374 | 19.064 | -19.425 | 6.344 | 1.00 | 41.47 |
| | ATOM | 544 | OD1 | ASP | A | 374 | 17.896 | -19.543 | 6.772 | 1.00 | 37.09 |
| 50 | ATOM | 545 | OD2 | ASP | A | 374 | 20.052 | -19.940 | 6.912 | 1.00 | 44.40 |
| | ATOM | 546 | C | ASP | A | 374 | 18.083 | -17.277 | 3.326 | 1.00 | 37.19 |
| | ATOM | 547 | O | ASP | A | 374 | 17.598 | -16.208 | 3.696 | 1.00 | 38.13 |
| | ATOM | 548 | N | GLN | A | 375 | 18.688 | -17.431 | 2.152 | 1.00 | 33.13 |
| | ATOM | 549 | CA | GLN | A | 375 | 18.788 | -16.339 | 1.198 | 1.00 | 31.94 |
| 55 | ATOM | 550 | CB | GLN | A | 375 | 19.634 | -16.756 | -0.001 | 1.00 | 28.81 |
| | ATOM | 551 | CG | GLN | A | 375 | 21.125 | -16.570 | 0.189 | 1.00 | 31.71 |
| | ATOM | 552 | CD | GLN | A | 375 | 21.920 | -17.222 | -0.922 | 1.00 | 34.49 |
| | ATOM | 553 | OE1 | GLN | A | 375 | 21.478 | -17.267 | -2.067 | 1.00 | 36.09 |
| | ATOM | 554 | NE2 | GLN | A | 375 | 23.097 | -17.736 | -0.588 | 1.00 | 40.32 |
| 60 | ATOM | 555 | C | GLN | A | 375 | 17.379 | -16.009 | 0.730 | 1.00 | 31.50 |
| | ATOM | 556 | O | GLN | A | 375 | 16.990 | -14.840 | 0.653 | 1.00 | 27.42 |

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|----|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 557 | N | VAL | A | 376 | 16.617 | -17.056 | 0.429 | 1.00 | 30.38 |
| | ATOM | 558 | CA | VAL | A | 376 | 15.242 | -16.907 | -0.027 | 1.00 | 33.50 |
| | ATOM | 559 | CB | VAL | A | 376 | 14.588 | -18.286 | -0.286 | 1.00 | 30.57 |
| | ATOM | 560 | CG1 | VAL | A | 376 | 13.093 | -18.122 | -0.516 | 1.00 | 33.14 |
| | ATOM | 561 | CG2 | VAL | A | 376 | 15.232 | -18.952 | -1.485 | 1.00 | 30.79 |
| 10 | ATOM | 562 | C | VAL | A | 376 | 14.393 | -16.159 | 1.002 | 1.00 | 33.80 |
| | ATOM | 563 | O | VAL | A | 376 | 13.653 | -15.237 | 0.661 | 1.00 | 34.89 |
| | ATOM | 564 | N | HIS | A | 377 | 14.500 | -16.568 | 2.261 | 1.00 | 33.35 |
| | ATOM | 565 | CA | HIS | A | 377 | 13.730 | -15.941 | 3.329 | 1.00 | 32.81 |
| | ATOM | 566 | CB | HIS | A | 377 | 13.966 | -16.694 | 4.644 | 1.00 | 35.24 |
| 15 | ATOM | 567 | CG | HIS | A | 377 | 13.429 | -15.989 | 5.851 | 1.00 | 40.15 |
| | ATOM | 568 | CD2 | HIS | A | 377 | 14.054 | -15.495 | 6.946 | 1.00 | 40.86 |
| | ATOM | 569 | ND1 | HIS | A | 377 | 12.090 | -15.703 | 6.012 | 1.00 | 43.08 |
| | ATOM | 570 | CE1 | HIS | A | 377 | 11.913 | -15.062 | 7.154 | 1.00 | 42.44 |
| | ATOM | 571 | NE2 | HIS | A | 377 | 13.089 | -14.922 | 7.740 | 1.00 | 44.85 |
| 20 | ATOM | 572 | C | HIS | A | 377 | 14.058 | -14.454 | 3.507 | 1.00 | 28.63 |
| | ATOM | 573 | O | HIS | A | 377 | 13.158 | -13.619 | 3.613 | 1.00 | 29.20 |
| | ATOM | 574 | N | LEU | A | 378 | 15.343 | -14.125 | 3.544 | 1.00 | 24.41 |
| | ATOM | 575 | CA | LEU | A | 378 | 15.759 | -12.738 | 3.721 | 1.00 | 23.21 |
| | ATOM | 576 | CB | LEU | A | 378 | 17.289 | -12.650 | 3.743 | 1.00 | 20.98 |
| 25 | ATOM | 577 | CG | LEU | A | 378 | 17.960 | -13.190 | 5.016 | 1.00 | 24.22 |
| | ATOM | 578 | CD1 | LEU | A | 378 | 19.471 | -13.041 | 4.924 | 1.00 | 21.07 |
| | ATOM | 579 | CD2 | LEU | A | 378 | 17.431 | -12.446 | 6.221 | 1.00 | 20.24 |
| | ATOM | 580 | C | LEU | A | 378 | 15.190 | -11.827 | 2.630 | 1.00 | 24.78 |
| | ATOM | 581 | O | LEU | A | 378 | 14.638 | -10.766 | 2.922 | 1.00 | 22.09 |
| 30 | ATOM | 582 | N | LEU | A | 379 | 15.321 | -12.242 | 1.374 | 1.00 | 24.13 |
| | ATOM | 583 | CA | LEU | A | 379 | 14.812 | -11.447 | 0.262 | 1.00 | 25.02 |
| | ATOM | 584 | CB | LEU | A | 379 | 15.307 | -12.025 | -1.062 | 1.00 | 27.12 |
| | ATOM | 585 | CG | LEU | A | 379 | 16.724 | -11.600 | -1.437 | 1.00 | 24.39 |
| | ATOM | 586 | CD1 | LEU | A | 379 | 17.299 | -12.557 | -2.470 | 1.00 | 27.58 |
| 35 | ATOM | 587 | CD2 | LEU | A | 379 | 16.679 | -10.178 | -1.983 | 1.00 | 29.05 |
| | ATOM | 588 | C | LEU | A | 379 | 13.287 | -11.355 | 0.246 | 1.00 | 27.61 |
| | ATOM | 589 | O | LEU | A | 379 | 12.726 | -10.301 | -0.062 | 1.00 | 26.16 |
| | ATOM | 590 | N | GLU | A | 380 | 12.616 | -12.454 | 0.576 | 1.00 | 25.65 |
| | ATOM | 591 | CA | GLU | A | 380 | 11.154 | -12.471 | 0.592 | 1.00 | 26.85 |
| 40 | ATOM | 592 | CB | GLU | A | 380 | 10.640 | -13.882 | 0.871 | 1.00 | 29.38 |
| | ATOM | 593 | CG | GLU | A | 380 | 10.718 | -14.796 | -0.331 | 1.00 | 35.58 |
| | ATOM | 594 | CD | GLU | A | 380 | 10.228 | -16.194 | -0.025 | 1.00 | 39.31 |
| | ATOM | 595 | OE1 | GLU | A | 380 | 10.142 | -17.008 | -0.967 | 1.00 | 42.89 |
| | ATOM | 596 | OE2 | GLU | A | 380 | 9.927 | -16.478 | 1.153 | 1.00 | 39.45 |
| 45 | ATOM | 597 | C | GLU | A | 380 | 10.604 | -11.526 | 1.649 | 1.00 | 25.43 |
| | ATOM | 598 | O | GLU | A | 380 | 9.551 | -10.925 | 1.469 | 1.00 | 27.75 |
| | ATOM | 599 | N | CYS | A | 381 | 11.324 | -11.400 | 2.753 | 1.00 | 25.57 |
| | ATOM | 600 | CA | CYS | A | 381 | 10.907 | -10.530 | 3.843 | 1.00 | 26.46 |
| | ATOM | 601 | CB | CYS | A | 381 | 11.570 | -11.000 | 5.149 | 1.00 | 31.46 |
| 50 | ATOM | 602 | SG | CYS | A | 381 | 11.305 | -9.946 | 6.623 | 1.00 | 45.32 |
| | ATOM | 603 | C | CYS | A | 381 | 11.262 | -9.059 | 3.589 | 1.00 | 24.77 |
| | ATOM | 604 | O | CYS | A | 381 | 10.516 | -8.166 | 3.975 | 1.00 | 25.01 |
| | ATOM | 605 | N | ALA | A | 382 | 12.377 | -8.815 | 2.903 | 1.00 | 22.23 |
| | ATOM | 606 | CA | ALA | A | 382 | 12.855 | -7.449 | 2.681 | 1.00 | 21.83 |
| 55 | ATOM | 607 | CB | ALA | A | 382 | 14.319 | -7.383 | 3.095 | 1.00 | 21.56 |
| | ATOM | 608 | C | ALA | A | 382 | 12.705 | -6.778 | 1.311 | 1.00 | 19.78 |
| | ATOM | 609 | O | ALA | A | 382 | 12.996 | -5.587 | 1.182 | 1.00 | 17.01 |
| | ATOM | 610 | N | TRP | A | 383 | 12.261 | -7.507 | 0.294 | 1.00 | 17.61 |
| | ATOM | 611 | CA | TRP | A | 383 | 12.164 | -6.915 | -1.036 | 1.00 | 18.06 |
| 60 | ATOM | 612 | CB | TRP | A | 383 | 11.580 | -7.928 | -2.035 | 1.00 | 20.28 |
| | ATOM | 613 | CG | TRP | A | 383 | 10.105 | -8.201 | -1.919 | 1.00 | 20.50 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 614 | CD2 | TRP | A | 383 | 9.049 | -7.509 | -2.599 | 1.00 | 22.48 |
| | ATOM | 615 | CE2 | TRP | A | 383 | 7.836 | -8.138 | -2.238 | 1.00 | 20.41 |
| | ATOM | 616 | CE3 | TRP | A | 383 | 9.012 | -6.420 | -3.482 | 1.00 | 22.06 |
| | ATOM | 617 | CD1 | TRP | A | 383 | 9.506 | -9.189 | -1.190 | 1.00 | 23.38 |
| | ATOM | 618 | NE1 | TRP | A | 383 | 8.142 | -9.159 | -1.377 | 1.00 | 22.59 |
| 10 | ATOM | 619 | CZ2 | TRP | A | 383 | 6.598 | -7.713 | -2.724 | 1.00 | 21.98 |
| | ATOM | 620 | CZ3 | TRP | A | 383 | 7.780 | -5.998 | -3.968 | 1.00 | 25.50 |
| | ATOM | 621 | CH2 | TRP | A | 383 | 6.589 | -6.647 | -3.587 | 1.00 | 23.11 |
| | ATOM | 622 | C | TRP | A | 383 | 11.448 | -5.564 | -1.170 | 1.00 | 19.18 |
| | ATOM | 623 | O | TRP | A | 383 | 11.972 | -4.663 | -1.824 | 1.00 | 19.27 |
| 15 | ATOM | 624 | N | LEU | A | 384 | 10.273 | -5.396 | -0.567 | 1.00 | 18.32 |
| | ATOM | 625 | CA | LEU | A | 384 | 9.586 | -4.118 | -0.719 | 1.00 | 16.38 |
| | ATOM | 626 | CB | LEU | A | 384 | 8.125 | -4.218 | -0.258 | 1.00 | 16.79 |
| | ATOM | 627 | CG | LEU | A | 384 | 7.211 | -3.013 | -0.577 | 1.00 | 18.39 |
| | ATOM | 628 | CD1 | LEU | A | 384 | 7.464 | -2.485 | -1.995 | 1.00 | 13.91 |
| 20 | ATOM | 629 | CD2 | LEU | A | 384 | 5.750 | -3.432 | -0.410 | 1.00 | 18.38 |
| | ATOM | 630 | C | LEU | A | 384 | 10.324 | -3.027 | 0.051 | 1.00 | 18.80 |
| | ATOM | 631 | O | LEU | A | 384 | 10.334 | -1.870 | -0.357 | 1.00 | 20.90 |
| | ATOM | 632 | N | GLU | A | 385 | 10.949 | -3.404 | 1.163 | 1.00 | 18.61 |
| | ATOM | 633 | CA | GLU | A | 385 | 11.718 | -2.462 | 1.970 | 1.00 | 19.58 |
| 25 | ATOM | 634 | CB | GLU | A | 385 | 12.274 | -3.154 | 3.213 | 1.00 | 17.43 |
| | ATOM | 635 | CG | GLU | A | 385 | 11.292 | -3.237 | 4.357 | 1.00 | 22.92 |
| | ATOM | 636 | CD | GLU | A | 385 | 11.963 | -3.676 | 5.640 | 1.00 | 25.83 |
| | ATOM | 637 | OE1 | GLU | A | 385 | 12.431 | -2.799 | 6.391 | 1.00 | 23.69 |
| | ATOM | 638 | OE2 | GLU | A | 385 | 12.027 | -4.897 | 5.889 | 1.00 | 27.64 |
| 30 | ATOM | 639 | C | GLU | A | 385 | 12.890 | -1.934 | 1.156 | 1.00 | 19.46 |
| | ATOM | 640 | O | GLU | A | 385 | 13.206 | -0.743 | 1.196 | 1.00 | 15.04 |
| | ATOM | 641 | N | ILE | A | 386 | 13.539 | -2.842 | 0.431 | 1.00 | 13.32 |
| | ATOM | 642 | CA | ILE | A | 386 | 14.685 | -2.484 | -0.388 | 1.00 | 15.01 |
| | ATOM | 643 | CB | ILE | A | 386 | 15.475 | -3.763 | -0.807 | 1.00 | 17.43 |
| 35 | ATOM | 644 | CG2 | ILE | A | 386 | 16.544 | -3.424 | -1.849 | 1.00 | 17.99 |
| | ATOM | 645 | CG1 | ILE | A | 386 | 16.185 | -4.338 | 0.432 | 1.00 | 20.31 |
| | ATOM | 646 | CD1 | ILE | A | 386 | 16.682 | -5.766 | 0.284 | 1.00 | 23.97 |
| | ATOM | 647 | C | ILE | A | 386 | 14.273 | -1.645 | -1.598 | 1.00 | 16.10 |
| | ATOM | 648 | O | ILE | A | 386 | 14.993 | -0.724 | -2.004 | 1.00 | 17.42 |
| 40 | ATOM | 649 | N | LEU | A | 387 | 13.112 | -1.944 | -2.167 | 1.00 | 17.61 |
| | ATOM | 650 | CA | LEU | A | 387 | 12.620 | -1.173 | -3.304 | 1.00 | 18.20 |
| | ATOM | 651 | CB | LEU | A | 387 | 11.359 | -1.814 | -3.882 | 1.00 | 17.51 |
| | ATOM | 652 | CG | LEU | A | 387 | 11.519 | -3.064 | -4.747 | 1.00 | 26.37 |
| | ATOM | 653 | CD1 | LEU | A | 387 | 10.173 | -3.406 | -5.395 | 1.00 | 24.63 |
| 45 | ATOM | 654 | CD2 | LEU | A | 387 | 12.589 | -2.824 | -5.808 | 1.00 | 21.58 |
| | ATOM | 655 | C | LEU | A | 387 | 12.283 | 0.249 | -2.838 | 1.00 | 17.60 |
| | ATOM | 656 | O | LEU | A | 387 | 12.571 | 1.224 | -3.530 | 1.00 | 17.15 |
| | ATOM | 657 | N | MET | A | 388 | 11.677 | 0.357 | -1.660 | 1.00 | 17.65 |
| | ATOM | 658 | CA | MET | A | 388 | 11.286 | 1.656 | -1.121 | 1.00 | 18.49 |
| 50 | ATOM | 659 | CB | MET | A | 388 | 10.302 | 1.460 | 0.034 | 1.00 | 19.65 |
| | ATOM | 660 | CG | MET | A | 388 | 8.893 | 1.105 | -0.435 | 1.00 | 15.12 |
| | ATOM | 661 | SD | MET | A | 388 | 7.744 | 0.769 | 0.910 | 1.00 | 18.73 |
| | ATOM | 662 | CE | MET | A | 388 | 6.163 | 0.908 | 0.048 | 1.00 | 18.34 |
| | ATOM | 663 | C | MET | A | 388 | 12.451 | 2.553 | -0.691 | 1.00 | 22.62 |
| 55 | ATOM | 664 | O | MET | A | 388 | 12.417 | 3.767 | -0.928 | 1.00 | 22.49 |
| | ATOM | 665 | N | ILE | A | 389 | 13.482 | 1.988 | -0.064 | 1.00 | 21.45 |
| | ATOM | 666 | CA | ILE | A | 389 | 14.604 | 2.831 | 0.331 | 1.00 | 18.54 |
| | ATOM | 667 | CB | ILE | A | 389 | 15.590 | 2.108 | 1.299 | 1.00 | 19.35 |
| | ATOM | 668 | CG2 | ILE | A | 389 | 16.362 | 0.998 | 0.578 | 1.00 | 15.50 |
| 60 | ATOM | 669 | CG1 | ILE | A | 389 | 16.556 | 3.142 | 1.889 | 1.00 | 21.95 |
| | ATOM | 670 | CD1 | ILE | A | 389 | 17.373 | 2.658 | 3.080 | 1.00 | 15.86 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 671 | C | ILE | A | 389 | 15.333 | 3.322 | -0.922 | 1.00 | 18.67 |
| | ATOM | 672 | O | ILE | A | 389 | 15.813 | 4.453 | -0.970 | 1.00 | 19.75 |
| | ATOM | 673 | N | GLY | A | 390 | 15.410 | 2.477 | -1.943 | 1.00 | 20.58 |
| | ATOM | 674 | CA | GLY | A | 390 | 16.049 | 2.895 | -3.183 | 1.00 | 19.33 |
| | ATOM | 675 | C | GLY | A | 390 | 15.243 | 4.021 | -3.819 | 1.00 | 17.48 |
| 10 | ATOM | 676 | O | GLY | A | 390 | 15.801 | 4.994 | -4.318 | 1.00 | 21.87 |
| | ATOM | 677 | N | LEU | A | 391 | 13.920 | 3.888 | -3.787 | 1.00 | 19.17 |
| | ATOM | 678 | CA | LEU | A | 391 | 13.018 | 4.887 | -4.343 | 1.00 | 21.50 |
| | ATOM | 679 | CB | LEU | A | 391 | 11.561 | 4.420 | -4.194 | 1.00 | 18.25 |
| | ATOM | 680 | CG | LEU | A | 391 | 10.480 | 5.497 | -4.342 | 1.00 | 21.98 |
| 15 | ATOM | 681 | CD1 | LEU | A | 391 | 10.579 | 6.156 | -5.725 | 1.00 | 21.39 |
| | ATOM | 682 | CD2 | LEU | A | 391 | 9.115 | 4.868 | -4.148 | 1.00 | 17.15 |
| | ATOM | 683 | C | LEU | A | 391 | 13.208 | 6.216 | -3.620 | 1.00 | 23.27 |
| | ATOM | 684 | O | LEU | A | 391 | 13.440 | 7.255 | -4.243 | 1.00 | 23.60 |
| | ATOM | 685 | N | VAL | A | 392 | 13.122 | 6.170 | -2.295 | 1.00 | 23.04 |
| 20 | ATOM | 686 | CA | VAL | A | 392 | 13.282 | 7.357 | -1.469 | 1.00 | 24.42 |
| | ATOM | 687 | CB | VAL | A | 392 | 13.186 | 6.993 | 0.042 | 1.00 | 27.38 |
| | ATOM | 688 | CG1 | VAL | A | 392 | 13.733 | 8.129 | 0.897 | 1.00 | 30.37 |
| | ATOM | 689 | CG2 | VAL | A | 392 | 11.739 | 6.712 | 0.414 | 1.00 | 23.48 |
| | ATOM | 690 | C | VAL | A | 392 | 14.626 | 8.014 | -1.754 | 1.00 | 27.55 |
| 25 | ATOM | 691 | O | VAL | A | 392 | 14.728 | 9.242 | -1.832 | 1.00 | 27.50 |
| | ATOM | 692 | N | TRP | A | 393 | 15.652 | 7.186 | -1.924 | 1.00 | 23.65 |
| | ATOM | 693 | CA | TRP | A | 393 | 16.999 | 7.670 | -2.204 | 1.00 | 24.76 |
| | ATOM | 694 | CB | TRP | A | 393 | 17.977 | 6.491 | -2.199 | 1.00 | 22.86 |
| | ATOM | 695 | CG | TRP | A | 393 | 19.287 | 6.784 | -2.857 | 1.00 | 25.90 |
| 30 | ATOM | 696 | CD2 | TRP | A | 393 | 20.341 | 7.605 | -2.339 | 1.00 | 28.09 |
| | ATOM | 697 | CE2 | TRP | A | 393 | 21.375 | 7.612 | -3.302 | 1.00 | 29.94 |
| | ATOM | 698 | CE3 | TRP | A | 393 | 20.512 | 8.335 | -1.154 | 1.00 | 30.20 |
| | ATOM | 699 | CD1 | TRP | A | 393 | 19.710 | 6.339 | -4.077 | 1.00 | 26.55 |
| | ATOM | 700 | NE1 | TRP | A | 393 | 20.963 | 6.833 | -4.351 | 1.00 | 30.64 |
| 35 | ATOM | 701 | CZ2 | TRP | A | 393 | 22.566 | 8.323 | -3.120 | 1.00 | 32.43 |
| | ATOM | 702 | CZ3 | TRP | A | 393 | 21.698 | 9.044 | -0.971 | 1.00 | 34.58 |
| | ATOM | 703 | CH2 | TRP | A | 393 | 22.709 | 9.030 | -1.950 | 1.00 | 36.54 |
| | ATOM | 704 | C | TRP | A | 393 | 17.082 | 8.414 | -3.547 | 1.00 | 25.02 |
| | ATOM | 705 | O | TRP | A | 393 | 17.767 | 9.435 | -3.650 | 1.00 | 20.97 |
| 40 | ATOM | 706 | N | ARG | A | 394 | 16.399 | 7.897 | -4.568 | 1.00 | 23.06 |
| | ATOM | 707 | CA | ARG | A | 394 | 16.412 | 8.531 | -5.890 | 1.00 | 25.97 |
| | ATOM | 708 | CB | ARG | A | 394 | 15.776 | 7.633 | -6.965 | 1.00 | 24.05 |
| | ATOM | 709 | CG | ARG | A | 394 | 16.243 | 6.195 | -7.024 | 1.00 | 26.05 |
| | ATOM | 710 | CD | ARG | A | 394 | 15.830 | 5.551 | -8.352 | 1.00 | 22.70 |
| 45 | ATOM | 711 | NE | ARG | A | 394 | 14.443 | 5.071 | -8.363 | 1.00 | 20.71 |
| | ATOM | 712 | CZ | ARG | A | 394 | 14.053 | 3.912 | -7.841 | 1.00 | 21.26 |
| | ATOM | 713 | NH1 | ARG | A | 394 | 14.944 | 3.108 | -7.267 | 1.00 | 20.09 |
| | ATOM | 714 | NH2 | ARG | A | 394 | 12.783 | 3.544 | -7.907 | 1.00 | 21.26 |
| | ATOM | 715 | C | ARG | A | 394 | 15.622 | 9.833 | -5.879 | 1.00 | 23.40 |
| 50 | ATOM | 716 | O | ARG | A | 394 | 15.889 | 10.729 | -6.677 | 1.00 | 28.61 |
| | ATOM | 717 | N | SER | A | 395 | 14.638 | 9.924 | -4.988 | 1.00 | 26.65 |
| | ATOM | 718 | CA | SER | A | 395 | 13.776 | 11.104 | -4.902 | 1.00 | 27.46 |
| | ATOM | 719 | CB | SER | A | 395 | 12.395 | 10.696 | -4.382 | 1.00 | 26.70 |
| | ATOM | 720 | OG | SER | A | 395 | 11.916 | 9.530 | -5.029 | 1.00 | 22.95 |
| 55 | ATOM | 721 | C | SER | A | 395 | 14.316 | 12.240 | -4.033 | 1.00 | 31.45 |
| | ATOM | 722 | O | SER | A | 395 | 13.726 | 13.324 | -3.977 | 1.00 | 28.11 |
| | ATOM | 723 | N | MET | A | 396 | 15.437 | 11.986 | -3.368 | 1.00 | 33.83 |
| | ATOM | 724 | CA | MET | A | 396 | 16.061 | 12.954 | -2.475 | 1.00 | 38.83 |
| | ATOM | 725 | CB | MET | A | 396 | 17.466 | 12.483 | -2.112 | 1.00 | 39.47 |
| 60 | ATOM | 726 | CG | MET | A | 396 | 17.585 | 11.919 | -0.715 | 1.00 | 41.37 |
| | ATOM | 727 | SD | MET | A | 396 | 19.192 | 12.262 | 0.004 | 1.00 | 42.20 |

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|----|------|-----|-----|-----|---|-----|--------|--------|---------|------|-------|
| 5 | ATOM | 728 | CE | MET | A | 396 | 20.263 | 11.996 | -1.404 | 1.00 | 42.84 |
| | ATOM | 729 | C | MET | A | 396 | 16.143 | 14.376 | -3.018 | 1.00 | 40.69 |
| | ATOM | 730 | O | MET | A | 396 | 15.637 | 15.316 | -2.403 | 1.00 | 38.85 |
| | ATOM | 731 | N | GLU | A | 397 | 16.794 | 14.526 | -4.166 | 1.00 | 42.19 |
| | ATOM | 732 | CA | GLU | A | 397 | 16.971 | 15.831 | -4.790 | 1.00 | 44.80 |
| 10 | ATOM | 733 | CB | GLU | A | 397 | 18.184 | 15.785 | -5.729 | 1.00 | 46.02 |
| | ATOM | 734 | CG | GLU | A | 397 | 17.883 | 15.189 | -7.096 | 1.00 | 54.42 |
| | ATOM | 735 | CD | GLU | A | 397 | 19.117 | 14.665 | -7.810 | 1.00 | 59.40 |
| | ATOM | 736 | OE1 | GLU | A | 397 | 19.219 | 13.430 | -7.990 | 1.00 | 60.63 |
| | ATOM | 737 | OE2 | GLU | A | 397 | 19.980 | 15.485 | -8.196 | 1.00 | 62.71 |
| 15 | ATOM | 738 | C | GLU | A | 397 | 15.735 | 16.322 | -5.554 | 1.00 | 42.94 |
| | ATOM | 739 | O | GLU | A | 397 | 15.830 | 17.229 | -6.376 | 1.00 | 44.68 |
| | ATOM | 740 | N | HIS | A | 398 | 14.579 | 15.728 | -5.280 | 1.00 | 40.82 |
| | ATOM | 741 | CA | HIS | A | 398 | 13.342 | 16.118 | -5.950 | 1.00 | 39.21 |
| | ATOM | 742 | CB | HIS | A | 398 | 12.924 | 15.043 | -6.956 | 1.00 | 39.05 |
| 20 | ATOM | 743 | CG | HIS | A | 398 | 13.870 | 14.886 | -8.104 | 1.00 | 41.57 |
| | ATOM | 744 | CD2 | HIS | A | 398 | 13.904 | 15.484 | -9.318 | 1.00 | 39.28 |
| | ATOM | 745 | ND1 | HIS | A | 398 | 14.940 | 14.017 | -8.074 | 1.00 | 41.85 |
| | ATOM | 746 | CE1 | HIS | A | 398 | 15.592 | 14.086 | -9.220 | 1.00 | 40.88 |
| | ATOM | 747 | NE2 | HIS | A | 398 | 14.985 | 14.969 | -9.993 | 1.00 | 42.30 |
| 25 | ATOM | 748 | C | HIS | A | 398 | 12.216 | 16.332 | -4.944 | 1.00 | 37.04 |
| | ATOM | 749 | O | HIS | A | 398 | 11.282 | 15.535 | -4.864 | 1.00 | 36.51 |
| | ATOM | 750 | N | PRO | A | 399 | 12.283 | 17.427 | -4.171 | 1.00 | 39.19 |
| | ATOM | 751 | CD | PRO | A | 399 | 13.328 | 18.467 | -4.198 | 1.00 | 35.36 |
| | ATOM | 752 | CA | PRO | A | 399 | 11.243 | 17.709 | -3.173 | 1.00 | 37.10 |
| 30 | ATOM | 753 | CB | PRO | A | 399 | 11.603 | 19.101 | -2.654 | 1.00 | 37.86 |
| | ATOM | 754 | CG | PRO | A | 399 | 13.050 | 19.267 | -2.963 | 1.00 | 35.83 |
| | ATOM | 755 | C | PRO | A | 399 | 9.828 | 17.663 | -3.744 | 1.00 | 37.02 |
| | ATOM | 756 | O | PRO | A | 399 | 9.554 | 18.249 | -4.789 | 1.00 | 38.52 |
| | ATOM | 757 | N | GLY | A | 400 | 8.938 | 16.954 | -3.057 | 1.00 | 33.58 |
| 35 | ATOM | 758 | CA | GLY | A | 400 | 7.559 | 16.865 | -3.503 | 1.00 | 32.12 |
| | ATOM | 759 | C | GLY | A | 400 | 7.230 | 15.706 | -4.428 | 1.00 | 32.43 |
| | ATOM | 760 | O | GLY | A | 400 | 6.063 | 15.344 | -4.574 | 1.00 | 33.21 |
| | ATOM | 761 | N | LYS | A | 401 | 8.237 | 15.112 | -5.055 | 1.00 | 31.35 |
| | ATOM | 762 | CA | LYS | A | 401 | 7.972 | 14.007 | -5.966 | 1.00 | 30.75 |
| 40 | ATOM | 763 | CB | LYS | A | 401 | 8.235 | 14.430 | -7.415 | 1.00 | 35.43 |
| | ATOM | 764 | CG | LYS | A | 401 | 8.130 | 15.927 | -7.675 | 1.00 | 35.15 |
| | ATOM | 765 | CD | LYS | A | 401 | 9.096 | 16.353 | -8.774 | 1.00 | 36.88 |
| | ATOM | 766 | CE | LYS | A | 401 | 8.733 | 17.721 | -9.331 | 1.00 | 36.71 |
| | ATOM | 767 | NZ | LYS | A | 401 | 7.295 | 18.027 | -9.116 | 1.00 | 34.22 |
| 45 | ATOM | 768 | C | LYS | A | 401 | 8.768 | 12.746 | -5.677 | 1.00 | 30.97 |
| | ATOM | 769 | O | LYS | A | 401 | 9.809 | 12.776 | -5.006 | 1.00 | 27.60 |
| | ATOM | 770 | N | LEU | A | 402 | 8.256 | 11.635 | -6.197 | 1.00 | 27.28 |
| | ATOM | 771 | CA | LEU | A | 402 | 8.889 | 10.334 | -6.050 | 1.00 | 29.07 |
| | ATOM | 772 | CB | LEU | A | 402 | 7.866 | 9.294 | -5.590 | 1.00 | 22.55 |
| 50 | ATOM | 773 | CG | LEU | A | 402 | 7.265 | 9.555 | -4.207 | 1.00 | 24.94 |
| | ATOM | 774 | CD1 | LEU | A | 402 | 6.126 | 8.583 | -3.937 | 1.00 | 19.32 |
| | ATOM | 775 | CD2 | LEU | A | 402 | 8.355 | 9.416 | -3.157 | 1.00 | 21.54 |
| | ATOM | 776 | C | LEU | A | 402 | 9.448 | 9.948 | -7.414 | 1.00 | 28.78 |
| | ATOM | 777 | O | LEU | A | 402 | 8.704 | 9.836 | -8.389 | 1.00 | 29.98 |
| 55 | ATOM | 778 | N | LEU | A | 403 | 10.761 | 9.770 | -7.487 | 1.00 | 27.57 |
| | ATOM | 779 | CA | LEU | A | 403 | 11.393 | 9.400 | -8.744 | 1.00 | 27.17 |
| | ATOM | 780 | CB | LEU | A | 403 | 12.825 | 9.937 | -8.816 | 1.00 | 26.95 |
| | ATOM | 781 | CG | LEU | A | 403 | 13.401 | 10.027 | -10.238 | 1.00 | 30.42 |
| | ATOM | 782 | CD1 | LEU | A | 403 | 14.519 | 11.046 | -10.288 | 1.00 | 30.76 |
| 60 | ATOM | 783 | CD2 | LEU | A | 403 | 13.915 | 8.665 | -10.676 | 1.00 | 33.11 |
| | ATOM | 784 | C | LEU | A | 403 | 11.419 | 7.891 | -8.901 | 1.00 | 24.78 |

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|----|------|-----|-----|-----|---|-----|--------|--------|---------|------|-------|
| 5 | ATOM | 785 | O | LEU | A | 403 | 12.428 | 7.257 | -8.619 | 1.00 | 24.68 |
| | ATOM | 786 | N | PHE | A | 404 | 10.306 | 7.319 | -9.344 | 1.00 | 23.11 |
| | ATOM | 787 | CA | PHE | A | 404 | 10.239 | 5.881 | -9.546 | 1.00 | 26.93 |
| | ATOM | 788 | CB | PHE | A | 404 | 8.826 | 5.470 | -9.946 | 1.00 | 27.04 |
| | ATOM | 789 | CG | PHE | A | 404 | 7.850 | 5.513 | -8.816 | 1.00 | 27.89 |
| 10 | ATOM | 790 | CD1 | PHE | A | 404 | 7.028 | 6.623 | -8.631 | 1.00 | 26.20 |
| | ATOM | 791 | CD2 | PHE | A | 404 | 7.750 | 4.444 | -7.925 | 1.00 | 23.10 |
| | ATOM | 792 | CE1 | PHE | A | 404 | 6.116 | 6.668 | -7.573 | 1.00 | 25.29 |
| | ATOM | 793 | CE2 | PHE | A | 404 | 6.845 | 4.481 | -6.870 | 1.00 | 21.01 |
| | ATOM | 794 | CZ | PHE | A | 404 | 6.026 | 5.595 | -6.693 | 1.00 | 22.91 |
| 15 | ATOM | 795 | C | PHE | A | 404 | 11.232 | 5.507 | -10.637 | 1.00 | 26.04 |
| | ATOM | 796 | O | PHE | A | 404 | 11.882 | 4.464 | -10.578 | 1.00 | 27.27 |
| | ATOM | 797 | N | ALA | A | 405 | 11.348 | 6.383 | -11.626 | 1.00 | 28.80 |
| | ATOM | 798 | CA | ALA | A | 405 | 12.271 | 6.195 | -12.740 | 1.00 | 29.21 |
| | ATOM | 799 | CB | ALA | A | 405 | 11.650 | 5.287 | -13.806 | 1.00 | 26.89 |
| 20 | ATOM | 800 | C | ALA | A | 405 | 12.549 | 7.578 | -13.317 | 1.00 | 30.23 |
| | ATOM | 801 | O | ALA | A | 405 | 11.770 | 8.508 | -13.109 | 1.00 | 27.38 |
| | ATOM | 802 | N | PRO | A | 406 | 13.672 | 7.737 | -14.032 | 1.00 | 30.05 |
| | ATOM | 803 | CD | PRO | A | 406 | 14.712 | 6.745 | -14.352 | 1.00 | 26.31 |
| | ATOM | 804 | CA | PRO | A | 406 | 13.977 | 9.053 | -14.604 | 1.00 | 32.10 |
| 25 | ATOM | 805 | CB | PRO | A | 406 | 15.232 | 8.800 | -15.438 | 1.00 | 31.28 |
| | ATOM | 806 | CG | PRO | A | 406 | 15.865 | 7.602 | -14.776 | 1.00 | 31.44 |
| | ATOM | 807 | C | PRO | A | 406 | 12.820 | 9.589 | -15.436 | 1.00 | 32.58 |
| | ATOM | 808 | O | PRO | A | 406 | 12.605 | 10.796 | -15.507 | 1.00 | 32.58 |
| | ATOM | 809 | N | ASN | A | 407 | 12.063 | 8.690 | -16.053 | 1.00 | 32.86 |
| 30 | ATOM | 810 | CA | ASN | A | 407 | 10.935 | 9.119 | -16.865 | 1.00 | 32.78 |
| | ATOM | 811 | CB | ASN | A | 407 | 10.950 | 8.418 | -18.228 | 1.00 | 34.73 |
| | ATOM | 812 | CG | ASN | A | 407 | 10.884 | 6.907 | -18.121 | 1.00 | 35.37 |
| | ATOM | 813 | OD1 | ASN | A | 407 | 11.189 | 6.317 | -17.077 | 1.00 | 30.24 |
| | ATOM | 814 | ND2 | ASN | A | 407 | 10.486 | 6.268 | -19.215 | 1.00 | 34.08 |
| 35 | ATOM | 815 | C | ASN | A | 407 | 9.605 | 8.901 | -16.166 | 1.00 | 34.90 |
| | ATOM | 816 | O | ASN | A | 407 | 8.549 | 8.897 | -16.798 | 1.00 | 36.09 |
| | ATOM | 817 | N | LEU | A | 408 | 9.660 | 8.724 | -14.851 | 1.00 | 33.56 |
| | ATOM | 818 | CA | LEU | A | 408 | 8.452 | 8.544 | -14.061 | 1.00 | 35.59 |
| | ATOM | 819 | CB | LEU | A | 408 | 8.141 | 7.062 | -13.851 | 1.00 | 33.81 |
| 40 | ATOM | 820 | CG | LEU | A | 408 | 6.696 | 6.823 | -13.397 | 1.00 | 36.44 |
| | ATOM | 821 | CD1 | LEU | A | 408 | 5.746 | 7.479 | -14.390 | 1.00 | 34.14 |
| | ATOM | 822 | CD2 | LEU | A | 408 | 6.406 | 5.334 | -13.287 | 1.00 | 32.96 |
| | ATOM | 823 | C | LEU | A | 408 | 8.607 | 9.245 | -12.717 | 1.00 | 38.03 |
| | ATOM | 824 | O | LEU | A | 408 | 8.880 | 8.614 | -11.695 | 1.00 | 36.38 |
| 45 | ATOM | 825 | N | LEU | A | 409 | 8.441 | 10.563 | -12.741 | 1.00 | 37.87 |
| | ATOM | 826 | CA | LEU | A | 409 | 8.548 | 11.395 | -11.553 | 1.00 | 37.95 |
| | ATOM | 827 | CB | LEU | A | 409 | 9.373 | 12.636 | -11.877 | 1.00 | 39.52 |
| | ATOM | 828 | CG | LEU | A | 409 | 10.023 | 13.399 | -10.728 | 1.00 | 42.46 |
| | ATOM | 829 | CD1 | LEU | A | 409 | 11.100 | 12.547 | -10.082 | 1.00 | 43.24 |
| 50 | ATOM | 830 | CD2 | LEU | A | 409 | 10.614 | 14.691 | -11.266 | 1.00 | 46.05 |
| | ATOM | 831 | C | LEU | A | 409 | 7.132 | 11.792 | -11.163 | 1.00 | 37.13 |
| | ATOM | 832 | O | LEU | A | 409 | 6.482 | 12.546 | -11.882 | 1.00 | 35.70 |
| | ATOM | 833 | N | LEU | A | 410 | 6.654 | 11.284 | -10.030 | 1.00 | 35.29 |
| | ATOM | 834 | CA | LEU | A | 410 | 5.297 | 11.576 | -9.583 | 1.00 | 33.33 |
| 55 | ATOM | 835 | CB | LEU | A | 410 | 4.503 | 10.277 | -9.449 | 1.00 | 29.37 |
| | ATOM | 836 | CG | LEU | A | 410 | 4.645 | 9.238 | -10.560 | 1.00 | 32.75 |
| | ATOM | 837 | CD1 | LEU | A | 410 | 4.026 | 7.925 | -10.104 | 1.00 | 29.16 |
| | ATOM | 838 | CD2 | LEU | A | 410 | 3.958 | 9.744 | -11.819 | 1.00 | 30.70 |
| | ATOM | 839 | C | LEU | A | 410 | 5.207 | 12.332 | -8.261 | 1.00 | 35.14 |
| 60 | ATOM | 840 | O | LEU | A | 410 | 6.078 | 12.214 | -7.400 | 1.00 | 36.94 |
| | ATOM | 841 | N | ASP | A | 411 | 4.141 | 13.108 | -8.105 | 1.00 | 34.76 |

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|----|------|-----|-----|-----|---|-----|--------|--------|---------|------|-------|
| 5 | ATOM | 842 | CA | ASP | A | 411 | 3.933 | 13.843 | -6.873 | 1.00 | 35.40 |
| | ATOM | 843 | CB | ASP | A | 411 | 3.733 | 15.341 | -7.144 | 1.00 | 40.02 |
| | ATOM | 844 | CG | ASP | A | 411 | 2.471 | 15.645 | -7.928 | 1.00 | 41.32 |
| | ATOM | 845 | OD1 | ASP | A | 411 | 1.570 | 14.785 | -8.001 | 1.00 | 45.03 |
| | ATOM | 846 | OD2 | ASP | A | 411 | 2.383 | 16.764 | -8.474 | 1.00 | 45.01 |
| 10 | ATOM | 847 | C | ASP | A | 411 | 2.727 | 13.234 | -6.179 | 1.00 | 36.10 |
| | ATOM | 848 | O | ASP | A | 411 | 2.033 | 12.395 | -6.762 | 1.00 | 34.08 |
| | ATOM | 849 | N | ARG | A | 412 | 2.480 | 13.647 | -4.940 | 1.00 | 35.99 |
| | ATOM | 850 | CA | ARG | A | 412 | 1.375 | 13.099 | -4.169 | 1.00 | 39.37 |
| | ATOM | 851 | CB | ARG | A | 412 | 1.260 | 13.824 | -2.825 | 1.00 | 39.75 |
| 15 | ATOM | 852 | CG | ARG | A | 412 | 0.562 | 15.168 | -2.870 | 1.00 | 40.49 |
| | ATOM | 853 | CD | ARG | A | 412 | 0.454 | 15.736 | -1.465 | 1.00 | 40.65 |
| | ATOM | 854 | NE | ARG | A | 412 | -0.261 | 14.826 | -0.577 | 1.00 | 37.48 |
| | ATOM | 855 | CZ | ARG | A | 412 | -1.574 | 14.855 | -0.384 | 1.00 | 42.84 |
| | ATOM | 856 | NH1 | ARG | A | 412 | -2.316 | 15.754 | -1.024 | 1.00 | 40.82 |
| 20 | ATOM | 857 | NH2 | ARG | A | 412 | -2.150 | 13.986 | 0.438 | 1.00 | 38.32 |
| | ATOM | 858 | C | ARG | A | 412 | 0.034 | 13.108 | -4.889 | 1.00 | 39.80 |
| | ATOM | 859 | O | ARG | A | 412 | -0.775 | 12.201 | -4.706 | 1.00 | 39.92 |
| | ATOM | 860 | N | ASN | A | 413 | -0.198 | 14.119 | -5.717 | 1.00 | 41.64 |
| | ATOM | 861 | CA | ASN | A | 413 | -1.458 | 14.215 | -6.440 | 1.00 | 43.19 |
| 25 | ATOM | 862 | CB | ASN | A | 413 | -1.518 | 15.533 | -7.210 | 1.00 | 46.44 |
| | ATOM | 863 | CG | ASN | A | 413 | -1.739 | 16.718 | -6.299 | 1.00 | 47.86 |
| | ATOM | 864 | OD1 | ASN | A | 413 | -2.376 | 16.594 | -5.249 | 1.00 | 48.05 |
| | ATOM | 865 | ND2 | ASN | A | 413 | -1.213 | 17.876 | -6.687 | 1.00 | 49.43 |
| | ATOM | 866 | C | ASN | A | 413 | -1.673 | 13.044 | -7.385 | 1.00 | 41.48 |
| 30 | ATOM | 867 | O | ASN | A | 413 | -2.792 | 12.567 | -7.546 | 1.00 | 40.50 |
| | ATOM | 868 | N | GLN | A | 414 | -0.600 | 12.577 | -8.010 | 1.00 | 42.82 |
| | ATOM | 869 | CA | GLN | A | 414 | -0.703 | 11.448 | -8.925 | 1.00 | 44.73 |
| | ATOM | 870 | CB | GLN | A | 414 | 0.585 | 11.307 | -9.741 | 1.00 | 47.52 |
| | ATOM | 871 | CG | GLN | A | 414 | 0.572 | 12.088 | -11.049 | 1.00 | 50.47 |
| 35 | ATOM | 872 | CD | GLN | A | 414 | 1.914 | 12.713 | -11.375 | 1.00 | 53.91 |
| | ATOM | 873 | OE1 | GLN | A | 414 | 2.591 | 13.257 | -10.501 | 1.00 | 53.68 |
| | ATOM | 874 | NE2 | GLN | A | 414 | 2.309 | 12.637 | -12.641 | 1.00 | 56.91 |
| | ATOM | 875 | C | GLN | A | 414 | -0.970 | 10.163 | -8.141 | 1.00 | 43.21 |
| | ATOM | 876 | O | GLN | A | 414 | -1.491 | 9.193 | -8.682 | 1.00 | 42.33 |
| 40 | ATOM | 877 | N | GLY | A | 415 | -0.618 | 10.168 | -6.860 | 1.00 | 41.97 |
| | ATOM | 878 | CA | GLY | A | 415 | -0.836 | 8.992 | -6.040 | 1.00 | 40.43 |
| | ATOM | 879 | C | GLY | A | 415 | -2.306 | 8.720 | -5.804 | 1.00 | 40.80 |
| | ATOM | 880 | O | GLY | A | 415 | -2.696 | 7.601 | -5.472 | 1.00 | 37.83 |
| | ATOM | 881 | N | LYS | A | 416 | -3.129 | 9.748 | -5.978 | 1.00 | 42.16 |
| 45 | ATOM | 882 | CA | LYS | A | 416 | -4.566 | 9.613 | -5.779 | 1.00 | 44.34 |
| | ATOM | 883 | CB | LYS | A | 416 | -5.212 | 10.996 | -5.704 | 1.00 | 45.65 |
| | ATOM | 884 | CG | LYS | A | 416 | -4.761 | 11.819 | -4.510 | 1.00 | 47.42 |
| | ATOM | 885 | CD | LYS | A | 416 | -4.910 | 13.309 | -4.777 | 1.00 | 50.97 |
| | ATOM | 886 | CE | LYS | A | 416 | -5.992 | 13.924 | -3.898 | 1.00 | 53.25 |
| 50 | ATOM | 887 | NZ | LYS | A | 416 | -5.416 | 14.764 | -2.809 | 1.00 | 56.95 |
| | ATOM | 888 | C | LYS | A | 416 | -5.227 | 8.793 | -6.886 | 1.00 | 45.33 |
| | ATOM | 889 | O | LYS | A | 416 | -6.339 | 8.299 | -6.714 | 1.00 | 46.50 |
| | ATOM | 890 | N | CYS | A | 417 | -4.540 | 8.648 | -8.015 | 1.00 | 45.18 |
| | ATOM | 891 | CA | CYS | A | 417 | -5.066 | 7.890 | -9.148 | 1.00 | 46.25 |
| 55 | ATOM | 892 | CB | CYS | A | 417 | -4.062 | 7.902 | -10.305 | 1.00 | 49.29 |
| | ATOM | 893 | SG | CYS | A | 417 | -3.916 | 9.493 | -11.168 | 1.00 | 49.59 |
| | ATOM | 894 | C | CYS | A | 417 | -5.373 | 6.452 | -8.752 | 1.00 | 47.18 |
| | ATOM | 895 | O | CYS | A | 417 | -6.220 | 5.794 | -9.359 | 1.00 | 46.50 |
| | ATOM | 896 | N | VAL | A | 418 | -4.671 | 5.968 | -7.731 | 1.00 | 45.07 |
| 60 | ATOM | 897 | CA | VAL | A | 418 | -4.866 | 4.612 | -7.232 | 1.00 | 42.75 |
| | ATOM | 898 | CB | VAL | A | 418 | -3.525 | 3.841 | -7.206 | 1.00 | 42.45 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|
| 5 | ATOM | 899 | CG1 | VAL | A | 418 | -3.670 | 2.563 | -6.410 | 1.00 | 40.22 |
| | ATOM | 900 | CG2 | VAL | A | 418 | -3.071 | 3.538 | -8.634 | 1.00 | 38.03 |
| | ATOM | 901 | C | VAL | A | 418 | -5.441 | 4.714 | -5.818 | 1.00 | 41.46 |
| | ATOM | 902 | O | VAL | A | 418 | -4.883 | 5.400 | -4.963 | 1.00 | 42.08 |
| 10 | ATOM | 903 | N | GLU | A | 419 | -6.559 | 4.036 | -5.579 | 1.00 | 40.95 |
| | ATOM | 904 | CA | GLU | A | 419 | -7.223 | 4.073 | -4.275 | 1.00 | 42.51 |
| | ATOM | 905 | CB | GLU | A | 419 | -8.536 | 3.282 | -4.333 | 1.00 | 44.52 |
| | ATOM | 906 | CG | GLU | A | 419 | -9.010 | 2.751 | -2.984 | 1.00 | 50.42 |
| | ATOM | 907 | CD | GLU | A | 419 | -10.413 | 2.168 | -3.035 | 1.00 | 54.38 |
| 15 | ATOM | 908 | OE1 | GLU | A | 419 | -10.582 | 1.059 | -3.590 | 1.00 | 54.09 |
| | ATOM | 909 | OE2 | GLU | A | 419 | -11.347 | 2.820 | -2.516 | 1.00 | 57.90 |
| | ATOM | 910 | C | GLU | A | 419 | -6.370 | 3.552 | -3.121 | 1.00 | 41.11 |
| | ATOM | 911 | O | GLU | A | 419 | -5.955 | 2.393 | -3.116 | 1.00 | 39.42 |
| | ATOM | 912 | N | GLY | A | 420 | -6.129 | 4.419 | -2.140 | 1.00 | 40.53 |
| 20 | ATOM | 913 | CA | GLY | A | 420 | -5.346 | 4.049 | -0.973 | 1.00 | 37.61 |
| | ATOM | 914 | C | GLY | A | 420 | -3.854 | 4.258 | -1.140 | 1.00 | 37.01 |
| | ATOM | 915 | O | GLY | A | 420 | -3.088 | 4.105 | -0.190 | 1.00 | 32.59 |
| | ATOM | 916 | N | MET | A | 421 | -3.444 | 4.623 | -2.350 | 1.00 | 36.21 |
| | ATOM | 917 | CA | MET | A | 421 | -2.035 | 4.825 | -2.656 | 1.00 | 36.02 |
| 25 | ATOM | 918 | CB | MET | A | 421 | -1.799 | 4.607 | -4.160 | 1.00 | 32.84 |
| | ATOM | 919 | CG | MET | A | 421 | -0.351 | 4.754 | -4.617 | 1.00 | 35.82 |
| | ATOM | 920 | SD | MET | A | 421 | 0.806 | 3.611 | -3.812 | 1.00 | 35.57 |
| | ATOM | 921 | CE | MET | A | 421 | 0.881 | 2.294 | -5.005 | 1.00 | 32.51 |
| | ATOM | 922 | C | MET | A | 421 | -1.474 | 6.180 | -2.226 | 1.00 | 34.93 |
| 30 | ATOM | 923 | O | MET | A | 421 | -0.275 | 6.294 | -1.985 | 1.00 | 35.17 |
| | ATOM | 924 | N | VAL | A | 422 | -2.319 | 7.205 | -2.118 | 1.00 | 33.97 |
| | ATOM | 925 | CA | VAL | A | 422 | -1.823 | 8.520 | -1.708 | 1.00 | 31.29 |
| | ATOM | 926 | CB | VAL | A | 422 | -2.927 | 9.607 | -1.766 | 1.00 | 33.14 |
| | ATOM | 927 | CG1 | VAL | A | 422 | -3.823 | 9.535 | -0.533 | 1.00 | 30.10 |
| 35 | ATOM | 928 | CG2 | VAL | A | 422 | -2.279 | 10.982 | -1.854 | 1.00 | 30.08 |
| | ATOM | 929 | C | VAL | A | 422 | -1.231 | 8.498 | -0.296 | 1.00 | 32.64 |
| | ATOM | 930 | O | VAL | A | 422 | -0.274 | 9.220 | 0.002 | 1.00 | 28.41 |
| | ATOM | 931 | N | GLU | A | 423 | -1.803 | 7.670 | 0.571 | 1.00 | 31.53 |
| | ATOM | 932 | CA | GLU | A | 423 | -1.311 | 7.558 | 1.935 | 1.00 | 35.99 |
| 40 | ATOM | 933 | CB | GLU | A | 423 | -2.190 | 6.594 | 2.737 | 1.00 | 40.37 |
| | ATOM | 934 | CG | GLU | A | 423 | -3.588 | 7.129 | 3.043 | 1.00 | 49.41 |
| | ATOM | 935 | CD | GLU | A | 423 | -4.438 | 7.336 | 1.795 | 1.00 | 52.38 |
| | ATOM | 936 | OE1 | GLU | A | 423 | -5.349 | 8.188 | 1.835 | 1.00 | 56.91 |
| | ATOM | 937 | OE2 | GLU | A | 423 | -4.200 | 6.652 | 0.776 | 1.00 | 54.53 |
| 45 | ATOM | 938 | C | GLU | A | 423 | 0.127 | 7.043 | 1.886 | 1.00 | 34.83 |
| | ATOM | 939 | O | GLU | A | 423 | 1.007 | 7.552 | 2.581 | 1.00 | 31.85 |
| | ATOM | 940 | N | ILE | A | 424 | 0.369 | 6.038 | 1.050 | 1.00 | 30.17 |
| | ATOM | 941 | CA | ILE | A | 424 | 1.711 | 5.488 | 0.929 | 1.00 | 28.99 |
| | ATOM | 942 | CB | ILE | A | 424 | 1.696 | 4.195 | 0.109 | 1.00 | 30.96 |
| 50 | ATOM | 943 | CG2 | ILE | A | 424 | 3.108 | 3.588 | 0.068 | 1.00 | 27.20 |
| | ATOM | 944 | CG1 | ILE | A | 424 | 0.671 | 3.230 | 0.725 | 1.00 | 30.77 |
| | ATOM | 945 | CD1 | ILE | A | 424 | 0.810 | 1.787 | 0.291 | 1.00 | 34.69 |
| | ATOM | 946 | C | ILE | A | 424 | 2.700 | 6.483 | 0.312 | 1.00 | 28.21 |
| | ATOM | 947 | O | ILE | A | 424 | 3.856 | 6.551 | 0.735 | 1.00 | 28.48 |
| 55 | ATOM | 948 | N | PHE | A | 425 | 2.253 | 7.260 | -0.675 | 1.00 | 27.68 |
| | ATOM | 949 | CA | PHE | A | 425 | 3.119 | 8.253 | -1.315 | 1.00 | 27.30 |
| | ATOM | 950 | CB | PHE | A | 425 | 2.381 | 8.958 | -2.458 | 1.00 | 26.36 |
| | ATOM | 951 | CG | PHE | A | 425 | 2.538 | 8.289 | -3.798 | 1.00 | 27.22 |
| | ATOM | 952 | CD1 | PHE | A | 425 | 2.619 | 9.050 | -4.958 | 1.00 | 27.36 |
| 60 | ATOM | 953 | CD2 | PHE | A | 425 | 2.566 | 6.900 | -3.905 | 1.00 | 27.89 |
| | ATOM | 954 | CE1 | PHE | A | 425 | 2.721 | 8.443 | -6.207 | 1.00 | 29.63 |
| | ATOM | 955 | CE2 | PHE | A | 425 | 2.668 | 6.282 | -5.149 | 1.00 | 27.28 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 956 | CZ | PHE | A | 425 | 2.745 | 7.056 | -6.303 | 1.00 | 27.63 |
| | ATOM | 957 | C | PHE | A | 425 | 3.591 | 9.306 | -0.312 | 1.00 | 25.66 |
| | ATOM | 958 | O | PHE | A | 425 | 4.757 | 9.713 | -0.328 | 1.00 | 26.33 |
| | ATOM | 959 | N | ASP | A | 426 | 2.680 | 9.746 | 0.552 | 1.00 | 27.92 |
| | ATOM | 960 | CA | ASP | A | 426 | 2.984 | 10.759 | 1.570 | 1.00 | 28.88 |
| 10 | ATOM | 961 | CB | ASP | A | 426 | 1.721 | 11.102 | 2.369 | 1.00 | 32.58 |
| | ATOM | 962 | CG | ASP | A | 426 | 0.781 | 12.034 | 1.613 | 1.00 | 37.47 |
| | ATOM | 963 | OD1 | ASP | A | 426 | -0.432 | 12.039 | 1.925 | 1.00 | 37.72 |
| | ATOM | 964 | OD2 | ASP | A | 426 | 1.253 | 12.758 | 0.710 | 1.00 | 36.35 |
| | ATOM | 965 | C | ASP | A | 426 | 4.071 | 10.278 | 2.532 | 1.00 | 26.96 |
| 15 | ATOM | 966 | O | ASP | A | 426 | 4.974 | 11.030 | 2.900 | 1.00 | 27.20 |
| | ATOM | 967 | N | MET | A | 427 | 3.978 | 9.022 | 2.947 | 1.00 | 25.76 |
| | ATOM | 968 | CA | MET | A | 427 | 4.981 | 8.468 | 3.856 | 1.00 | 25.89 |
| | ATOM | 969 | CB | MET | A | 427 | 4.567 | 7.070 | 4.309 | 1.00 | 21.17 |
| | ATOM | 970 | CG | MET | A | 427 | 3.385 | 7.072 | 5.257 | 1.00 | 24.38 |
| 20 | ATOM | 971 | SD | MET | A | 427 | 3.153 | 5.489 | 6.080 | 1.00 | 34.32 |
| | ATOM | 972 | CE | MET | A | 427 | 2.173 | 4.637 | 4.910 | 1.00 | 21.03 |
| | ATOM | 973 | C | MET | A | 427 | 6.321 | 8.410 | 3.128 | 1.00 | 22.29 |
| | ATOM | 974 | O | MET | A | 427 | 7.363 | 8.760 | 3.689 | 1.00 | 22.19 |
| | ATOM | 975 | N | LEU | A | 428 | 6.285 | 7.985 | 1.868 | 1.00 | 21.75 |
| 25 | ATOM | 976 | CA | LEU | A | 428 | 7.506 | 7.892 | 1.075 | 1.00 | 22.91 |
| | ATOM | 977 | CB | LEU | A | 428 | 7.202 | 7.252 | -0.287 | 1.00 | 18.47 |
| | ATOM | 978 | CG | LEU | A | 428 | 6.910 | 5.747 | -0.176 | 1.00 | 19.24 |
| | ATOM | 979 | CD1 | LEU | A | 428 | 6.278 | 5.222 | -1.468 | 1.00 | 16.82 |
| | ATOM | 980 | CD2 | LEU | A | 428 | 8.204 | 5.010 | 0.131 | 1.00 | 16.23 |
| 30 | ATOM | 981 | C | LEU | A | 428 | 8.148 | 9.269 | 0.902 | 1.00 | 23.98 |
| | ATOM | 982 | O | LEU | A | 428 | 9.366 | 9.416 | 1.034 | 1.00 | 23.06 |
| | ATOM | 983 | N | LEU | A | 429 | 7.328 | 10.281 | 0.628 | 1.00 | 23.91 |
| | ATOM | 984 | CA | LEU | A | 429 | 7.837 | 11.642 | 0.462 | 1.00 | 26.29 |
| | ATOM | 985 | CB | LEU | A | 429 | 6.714 | 12.571 | -0.003 | 1.00 | 27.47 |
| 35 | ATOM | 986 | CG | LEU | A | 429 | 6.331 | 12.411 | -1.476 | 1.00 | 30.78 |
| | ATOM | 987 | CD1 | LEU | A | 429 | 5.022 | 13.139 | -1.751 | 1.00 | 34.75 |
| | ATOM | 988 | CD2 | LEU | A | 429 | 7.449 | 12.952 | -2.350 | 1.00 | 31.96 |
| | ATOM | 989 | C | LEU | A | 429 | 8.425 | 12.166 | 1.776 | 1.00 | 25.83 |
| | ATOM | 990 | O | LEU | A | 429 | 9.482 | 12.808 | 1.793 | 1.00 | 26.42 |
| 40 | ATOM | 991 | N | ALA | A | 430 | 7.734 | 11.890 | 2.877 | 1.00 | 26.45 |
| | ATOM | 992 | CA | ALA | A | 430 | 8.201 | 12.333 | 4.185 | 1.00 | 26.11 |
| | ATOM | 993 | CB | ALA | A | 430 | 7.214 | 11.909 | 5.265 | 1.00 | 23.13 |
| | ATOM | 994 | C | ALA | A | 430 | 9.577 | 11.742 | 4.462 | 1.00 | 25.01 |
| | ATOM | 995 | O | ALA | A | 430 | 10.455 | 12.409 | 5.005 | 1.00 | 24.31 |
| 45 | ATOM | 996 | N | THR | A | 431 | 9.767 | 10.486 | 4.074 | 1.00 | 25.25 |
| | ATOM | 997 | CA | THR | A | 431 | 11.046 | 9.825 | 4.294 | 1.00 | 22.78 |
| | ATOM | 998 | CB | THR | A | 431 | 10.973 | 8.323 | 3.962 | 1.00 | 21.36 |
| | ATOM | 999 | OG1 | THR | A | 431 | 9.924 | 7.727 | 4.727 | 1.00 | 20.27 |
| | ATOM | 1000 | CG2 | THR | A | 431 | 12.291 | 7.633 | 4.299 | 1.00 | 19.99 |
| 50 | ATOM | 1001 | C | THR | A | 431 | 12.103 | 10.477 | 3.429 | 1.00 | 23.73 |
| | ATOM | 1002 | O | THR | A | 431 | 13.234 | 10.667 | 3.868 | 1.00 | 19.60 |
| | ATOM | 1003 | N | SER | A | 432 | 11.736 | 10.819 | 2.197 | 1.00 | 24.32 |
| | ATOM | 1004 | CA | SER | A | 432 | 12.676 | 11.479 | 1.301 | 1.00 | 26.96 |
| | ATOM | 1005 | CB | SER | A | 432 | 12.067 | 11.650 | -0.093 | 1.00 | 28.70 |
| 55 | ATOM | 1006 | OG | SER | A | 432 | 13.084 | 11.930 | -1.039 | 1.00 | 33.42 |
| | ATOM | 1007 | C | SER | A | 432 | 13.033 | 12.850 | 1.876 | 1.00 | 27.92 |
| | ATOM | 1008 | O | SER | A | 432 | 14.176 | 13.294 | 1.779 | 1.00 | 30.78 |
| | ATOM | 1009 | N | SER | A | 433 | 12.045 | 13.521 | 2.459 | 1.00 | 28.96 |
| | ATOM | 1010 | CA | SER | A | 433 | 12.269 | 14.824 | 3.076 | 1.00 | 34.21 |
| 60 | ATOM | 1011 | CB | SER | A | 433 | 10.957 | 15.387 | 3.623 | 1.00 | 35.07 |
| | ATOM | 1012 | OG | SER | A | 433 | 10.175 | 15.961 | 2.591 | 1.00 | 42.38 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1013 | C | SER | A | 433 | 13.263 | 14.644 | 4.223 | 1.00 | 33.43 |
| | ATOM | 1014 | O | SER | A | 433 | 14.152 | 15.473 | 4.429 | 1.00 | 31.94 |
| | ATOM | 1015 | N | ARG | A | 434 | 13.105 | 13.545 | 4.959 | 1.00 | 31.32 |
| | ATOM | 1016 | CA | ARG | A | 434 | 13.980 | 13.236 | 6.086 | 1.00 | 29.78 |
| | ATOM | 1017 | CB | ARG | A | 434 | 13.468 | 11.994 | 6.819 | 1.00 | 29.84 |
| 10 | ATOM | 1018 | CG | ARG | A | 434 | 14.331 | 11.541 | 7.983 | 1.00 | 32.17 |
| | ATOM | 1019 | CD | ARG | A | 434 | 14.626 | 12.672 | 8.958 | 1.00 | 37.00 |
| | ATOM | 1020 | NE | ARG | A | 434 | 15.321 | 12.169 | 10.140 | 1.00 | 39.44 |
| | ATOM | 1021 | CZ | ARG | A | 434 | 15.935 | 12.935 | 11.034 | 1.00 | 44.06 |
| | ATOM | 1022 | NH1 | ARG | A | 434 | 15.949 | 14.255 | 10.885 | 1.00 | 45.52 |
| 15 | ATOM | 1023 | NH2 | ARG | A | 434 | 16.528 | 12.381 | 12.084 | 1.00 | 45.01 |
| | ATOM | 1024 | C | ARG | A | 434 | 15.413 | 13.014 | 5.605 | 1.00 | 29.24 |
| | ATOM | 1025 | O | ARG | A | 434 | 16.352 | 13.563 | 6.173 | 1.00 | 29.72 |
| | ATOM | 1026 | N | PHE | A | 435 | 15.577 | 12.206 | 4.561 | 1.00 | 28.95 |
| | ATOM | 1027 | CA | PHE | A | 435 | 16.901 | 11.935 | 4.000 | 1.00 | 30.59 |
| 20 | ATOM | 1028 | CB | PHE | A | 435 | 16.777 | 11.045 | 2.758 | 1.00 | 32.03 |
| | ATOM | 1029 | CG | PHE | A | 435 | 16.795 | 9.563 | 3.051 | 1.00 | 31.88 |
| | ATOM | 1030 | CD1 | PHE | A | 435 | 16.758 | 9.084 | 4.359 | 1.00 | 35.60 |
| | ATOM | 1031 | CD2 | PHE | A | 435 | 16.847 | 8.643 | 2.009 | 1.00 | 35.89 |
| | ATOM | 1032 | CE1 | PHE | A | 435 | 16.771 | 7.709 | 4.622 | 1.00 | 35.36 |
| 25 | ATOM | 1033 | CE2 | PHE | A | 435 | 16.860 | 7.271 | 2.262 | 1.00 | 32.71 |
| | ATOM | 1034 | CZ | PHE | A | 435 | 16.821 | 6.807 | 3.570 | 1.00 | 33.24 |
| | ATOM | 1035 | C | PHE | A | 435 | 17.576 | 13.253 | 3.607 | 1.00 | 32.73 |
| | ATOM | 1036 | O | PHE | A | 435 | 18.763 | 13.464 | 3.871 | 1.00 | 31.16 |
| | ATOM | 1037 | N | ARG | A | 436 | 16.812 | 14.137 | 2.975 | 1.00 | 33.37 |
| 30 | ATOM | 1038 | CA | ARG | A | 436 | 17.341 | 15.429 | 2.549 | 1.00 | 39.13 |
| | ATOM | 1039 | CB | ARG | A | 436 | 16.282 | 16.206 | 1.756 | 1.00 | 40.42 |
| | ATOM | 1040 | CG | ARG | A | 436 | 16.846 | 17.317 | 0.877 | 1.00 | 43.09 |
| | ATOM | 1041 | CD | ARG | A | 436 | 15.750 | 17.960 | 0.040 | 1.00 | 44.53 |
| | ATOM | 1042 | NE | ARG | A | 436 | 14.826 | 16.955 | -0.472 | 1.00 | 48.34 |
| 35 | ATOM | 1043 | CZ | ARG | A | 436 | 13.530 | 16.913 | -0.184 | 1.00 | 48.81 |
| | ATOM | 1044 | NH1 | ARG | A | 436 | 12.997 | 17.823 | 0.619 | 1.00 | 47.80 |
| | ATOM | 1045 | NH2 | ARG | A | 436 | 12.769 | 15.950 | -0.687 | 1.00 | 49.53 |
| | ATOM | 1046 | C | ARG | A | 436 | 17.792 | 16.250 | 3.753 | 1.00 | 38.10 |
| | ATOM | 1047 | O | ARG | A | 436 | 18.896 | 16.789 | 3.764 | 1.00 | 41.00 |
| 40 | ATOM | 1048 | N | MET | A | 437 | 16.936 | 16.334 | 4.766 | 1.00 | 39.47 |
| | ATOM | 1049 | CA | MET | A | 437 | 17.257 | 17.087 | 5.975 | 1.00 | 38.20 |
| | ATOM | 1050 | CB | MET | A | 437 | 16.102 | 16.998 | 6.965 | 1.00 | 39.79 |
| | ATOM | 1051 | C | MET | A | 437 | 18.550 | 16.594 | 6.626 | 1.00 | 41.15 |
| | ATOM | 1052 | O | MET | A | 437 | 19.303 | 17.378 | 7.201 | 1.00 | 40.20 |
| 45 | ATOM | 1053 | N | MET | A | 438 | 18.804 | 15.285 | 6.538 | 1.00 | 39.65 |
| | ATOM | 1054 | CA | MET | A | 438 | 20.011 | 14.693 | 7.117 | 1.00 | 39.70 |
| | ATOM | 1055 | CB | MET | A | 438 | 19.787 | 13.221 | 7.463 | 1.00 | 39.90 |
| | ATOM | 1056 | CG | MET | A | 438 | 18.694 | 12.938 | 8.460 | 1.00 | 41.94 |
| | ATOM | 1057 | SD | MET | A | 438 | 18.747 | 11.188 | 8.880 | 1.00 | 43.12 |
| 50 | ATOM | 1058 | CE | MET | A | 438 | 20.374 | 11.064 | 9.619 | 1.00 | 43.73 |
| | ATOM | 1059 | C | MET | A | 438 | 21.176 | 14.756 | 6.142 | 1.00 | 38.03 |
| | ATOM | 1060 | O | MET | A | 438 | 22.321 | 14.503 | 6.522 | 1.00 | 38.39 |
| | ATOM | 1061 | N | ASN | A | 439 | 20.886 | 15.070 | 4.895 | 1.00 | 37.64 |
| | ATOM | 1062 | CA | ASN | A | 439 | 21.924 | 15.118 | 3.895 | 1.00 | 35.68 |
| 55 | ATOM | 1063 | CB | ASN | A | 439 | 23.019 | 16.125 | 4.243 | 1.00 | 40.98 |
| | ATOM | 1064 | CG | ASN | A | 439 | 23.933 | 16.407 | 3.090 | 1.00 | 45.09 |
| | ATOM | 1065 | OD1 | ASN | A | 439 | 23.528 | 16.295 | 1.934 | 1.00 | 47.16 |
| | ATOM | 1066 | ND2 | ASN | A | 439 | 25.197 | 16.733 | 3.372 | 1.00 | 46.87 |
| | ATOM | 1067 | C | ASN | A | 439 | 22.552 | 13.732 | 3.739 | 1.00 | 31.06 |
| 60 | ATOM | 1068 | O | ASN | A | 439 | 23.764 | 13.581 | 3.649 | 1.00 | 29.54 |
| | ATOM | 1069 | N | LEU | A | 440 | 21.692 | 12.698 | 3.704 | 1.00 | 31.47 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1070 | CA | LEU | A | 440 | 22.161 | 11.326 | 3.579 | 1.00 | 31.63 |
| | ATOM | 1071 | CB | LEU | A | 440 | 20.991 | 10.344 | 3.380 | 1.00 | 33.05 |
| | ATOM | 1072 | CG | LEU | A | 440 | 21.451 | 8.886 | 3.209 | 1.00 | 37.07 |
| | ATOM | 1073 | CD1 | LEU | A | 440 | 21.957 | 8.353 | 4.546 | 1.00 | 36.18 |
| | ATOM | 1074 | CD2 | LEU | A | 440 | 20.318 | 8.032 | 2.682 | 1.00 | 32.33 |
| 10 | ATOM | 1075 | C | LEU | A | 440 | 23.146 | 11.161 | 2.435 | 1.00 | 32.10 |
| | ATOM | 1076 | O | LEU | A | 440 | 22.925 | 11.671 | 1.333 | 1.00 | 32.76 |
| | ATOM | 1077 | N | GLN | A | 441 | 24.225 | 10.450 | 2.702 | 1.00 | 32.54 |
| | ATOM | 1078 | CA | GLN | A | 441 | 25.255 | 10.220 | 1.699 | 1.00 | 31.97 |
| | ATOM | 1079 | CB | GLN | A | 441 | 26.632 | 10.320 | 2.345 | 1.00 | 31.75 |
| 15 | ATOM | 1080 | CG | GLN | A | 441 | 26.896 | 11.669 | 2.979 | 1.00 | 35.56 |
| | ATOM | 1081 | CD | GLN | A | 441 | 27.040 | 12.748 | 1.939 | 1.00 | 34.97 |
| | ATOM | 1082 | OE1 | GLN | A | 441 | 27.985 | 12.782 | 1.167 | 1.00 | 35.51 |
| | ATOM | 1083 | NE2 | GLN | A | 441 | 26.053 | 13.659 | 1.899 | 1.00 | 35.41 |
| | ATOM | 1084 | C | GLN | A | 441 | 25.100 | 8.860 | 1.038 | 1.00 | 34.08 |
| 20 | ATOM | 1085 | O | GLN | A | 441 | 24.540 | 7.931 | 1.625 | 1.00 | 30.73 |
| | ATOM | 1086 | N | GLY | A | 442 | 25.608 | 8.752 | -0.187 | 1.00 | 32.78 |
| | ATOM | 1087 | CA | GLY | A | 442 | 25.528 | 7.503 | -0.921 | 1.00 | 32.91 |
| | ATOM | 1088 | C | GLY | A | 442 | 26.181 | 6.350 | -0.184 | 1.00 | 31.87 |
| | ATOM | 1089 | O | GLY | A | 442 | 25.642 | 5.245 | -0.154 | 1.00 | 33.18 |
| 25 | ATOM | 1090 | N | GLU | A | 443 | 27.340 | 6.603 | 0.416 | 1.00 | 30.60 |
| | ATOM | 1091 | CA | GLU | A | 443 | 28.057 | 5.567 | 1.150 | 1.00 | 30.85 |
| | ATOM | 1092 | CB | GLU | A | 443 | 29.376 | 6.111 | 1.704 | 1.00 | 32.74 |
| | ATOM | 1093 | CG | GLU | A | 443 | 30.425 | 6.378 | 0.646 | 1.00 | 36.30 |
| | ATOM | 1094 | CD | GLU | A | 443 | 30.310 | 7.770 | 0.066 | 1.00 | 40.92 |
| 30 | ATOM | 1095 | OE1 | GLU | A | 443 | 29.677 | 8.630 | 0.716 | 1.00 | 42.27 |
| | ATOM | 1096 | OE2 | GLU | A | 443 | 30.853 | 8.003 | -1.038 | 1.00 | 46.82 |
| | ATOM | 1097 | C | GLU | A | 443 | 27.206 | 5.048 | 2.299 | 1.00 | 30.43 |
| | ATOM | 1098 | O | GLU | A | 443 | 27.211 | 3.854 | 2.595 | 1.00 | 28.11 |
| | ATOM | 1099 | N | GLU | A | 444 | 26.482 | 5.955 | 2.948 | 1.00 | 30.26 |
| 35 | ATOM | 1100 | CA | GLU | A | 444 | 25.619 | 5.589 | 4.067 | 1.00 | 28.18 |
| | ATOM | 1101 | CB | GLU | A | 444 | 25.147 | 6.843 | 4.797 | 1.00 | 26.32 |
| | ATOM | 1102 | CG | GLU | A | 444 | 26.250 | 7.633 | 5.463 | 1.00 | 29.27 |
| | ATOM | 1103 | CD | GLU | A | 444 | 25.748 | 8.944 | 6.023 | 1.00 | 29.62 |
| | ATOM | 1104 | OE1 | GLU | A | 444 | 25.006 | 9.652 | 5.304 | 1.00 | 32.00 |
| 40 | ATOM | 1105 | OE2 | GLU | A | 444 | 26.088 | 9.268 | 7.182 | 1.00 | 29.02 |
| | ATOM | 1106 | C | GLU | A | 444 | 24.403 | 4.813 | 3.572 | 1.00 | 26.93 |
| | ATOM | 1107 | O | GLU | A | 444 | 23.970 | 3.841 | 4.191 | 1.00 | 24.78 |
| | ATOM | 1108 | N | PHE | A | 445 | 23.861 | 5.256 | 2.443 | 1.00 | 27.79 |
| | ATOM | 1109 | CA | PHE | A | 445 | 22.688 | 4.633 | 1.853 | 1.00 | 24.50 |
| 45 | ATOM | 1110 | CB | PHE | A | 445 | 22.254 | 5.416 | 0.610 | 1.00 | 25.40 |
| | ATOM | 1111 | CG | PHE | A | 445 | 21.372 | 4.634 | -0.316 | 1.00 | 23.74 |
| | ATOM | 1112 | CD1 | PHE | A | 445 | 20.034 | 4.419 | -0.004 | 1.00 | 23.00 |
| | ATOM | 1113 | CD2 | PHE | A | 445 | 21.885 | 4.094 | -1.489 | 1.00 | 22.37 |
| | ATOM | 1114 | CE1 | PHE | A | 445 | 19.215 | 3.670 | -0.855 | 1.00 | 22.57 |
| 50 | ATOM | 1115 | CE2 | PHE | A | 445 | 21.079 | 3.349 | -2.342 | 1.00 | 21.69 |
| | ATOM | 1116 | CZ | PHE | A | 445 | 19.741 | 3.138 | -2.023 | 1.00 | 22.25 |
| | ATOM | 1117 | C | PHE | A | 445 | 22.913 | 3.169 | 1.489 | 1.00 | 22.81 |
| | ATOM | 1118 | O | PHE | A | 445 | 22.083 | 2.316 | 1.796 | 1.00 | 22.92 |
| | ATOM | 1119 | N | VAL | A | 446 | 24.019 | 2.868 | 0.822 | 1.00 | 22.46 |
| 55 | ATOM | 1120 | CA | VAL | A | 446 | 24.278 | 1.481 | 0.447 | 1.00 | 22.26 |
| | ATOM | 1121 | CB | VAL | A | 446 | 25.522 | 1.360 | -0.465 | 1.00 | 22.87 |
| | ATOM | 1122 | CG1 | VAL | A | 446 | 25.251 | 2.046 | -1.799 | 1.00 | 22.57 |
| | ATOM | 1123 | CG2 | VAL | A | 446 | 26.735 | 1.968 | 0.217 | 1.00 | 22.38 |
| | ATOM | 1124 | C | VAL | A | 446 | 24.467 | 0.614 | 1.694 | 1.00 | 23.68 |
| 60 | ATOM | 1125 | O | VAL | A | 446 | 24.177 | -0.586 | 1.680 | 1.00 | 22.91 |
| | ATOM | 1126 | N | CYS | A | 447 | 24.962 | 1.223 | 2.770 | 1.00 | 22.02 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1127 | CA | CYS | A | 447 | 25.155 | 0.503 | 4.025 | 1.00 | 24.17 |
| | ATOM | 1128 | CB | CYS | A | 447 | 25.953 | 1.359 | 5.011 | 1.00 | 23.95 |
| | ATOM | 1129 | SG | CYS | A | 447 | 27.738 | 1.324 | 4.731 | 1.00 | 28.57 |
| | ATOM | 1130 | C | CYS | A | 447 | 23.781 | 0.178 | 4.618 | 1.00 | 21.14 |
| | ATOM | 1131 | O | CYS | A | 447 | 23.512 | -0.960 | 5.002 | 1.00 | 19.37 |
| 10 | ATOM | 1132 | N | LEU | A | 448 | 22.915 | 1.186 | 4.680 | 1.00 | 19.28 |
| | ATOM | 1133 | CA | LEU | A | 448 | 21.568 | 1.002 | 5.219 | 1.00 | 21.31 |
| | ATOM | 1134 | CB | LEU | A | 448 | 20.803 | 2.324 | 5.207 | 1.00 | 21.90 |
| | ATOM | 1135 | CG | LEU | A | 448 | 21.142 | 3.337 | 6.303 | 1.00 | 26.61 |
| | ATOM | 1136 | CD1 | LEU | A | 448 | 20.328 | 4.594 | 6.072 | 1.00 | 27.74 |
| 15 | ATOM | 1137 | CD2 | LEU | A | 448 | 20.827 | 2.760 | 7.672 | 1.00 | 24.03 |
| | ATOM | 1138 | C | LEU | A | 448 | 20.766 | -0.038 | 4.442 | 1.00 | 21.72 |
| | ATOM | 1139 | O | LEU | A | 448 | 20.006 | -0.803 | 5.030 | 1.00 | 20.87 |
| | ATOM | 1140 | N | LYS | A | 449 | 20.929 | -0.055 | 3.119 | 1.00 | 21.42 |
| 20 | ATOM | 1141 | CA | LYS | A | 449 | 20.205 | -0.997 | 2.269 | 1.00 | 20.98 |
| | ATOM | 1142 | CB | LYS | A | 449 | 20.440 | -0.659 | 0.788 | 1.00 | 21.55 |
| | ATOM | 1143 | CG | LYS | A | 449 | 19.438 | -1.297 | -0.173 | 1.00 | 24.82 |
| | ATOM | 1144 | CD | LYS | A | 449 | 19.456 | -0.613 | -1.542 | 1.00 | 23.33 |
| | ATOM | 1145 | CE | LYS | A | 449 | 20.816 | -0.754 | -2.229 | 1.00 | 23.58 |
| | ATOM | 1146 | NZ | LYS | A | 449 | 20.741 | -0.482 | -3.698 | 1.00 | 28.77 |
| 25 | ATOM | 1147 | C | LYS | A | 449 | 20.629 | -2.436 | 2.548 | 1.00 | 20.33 |
| | ATOM | 1148 | O | LYS | A | 449 | 19.800 | -3.345 | 2.552 | 1.00 | 20.57 |
| | ATOM | 1149 | N | SER | A | 450 | 21.924 | -2.637 | 2.777 | 1.00 | 19.25 |
| | ATOM | 1150 | CA | SER | A | 450 | 22.451 | -3.965 | 3.074 | 1.00 | 21.84 |
| | ATOM | 1151 | CB | SER | A | 450 | 23.982 | -3.953 | 3.041 | 1.00 | 20.59 |
| 30 | ATOM | 1152 | OG | SER | A | 450 | 24.460 | -3.975 | 1.702 | 1.00 | 29.78 |
| | ATOM | 1153 | C | SER | A | 450 | 21.975 | -4.408 | 4.454 | 1.00 | 21.58 |
| | ATOM | 1154 | O | SER | A | 450 | 21.728 | -5.590 | 4.682 | 1.00 | 20.06 |
| | ATOM | 1155 | N | ILE | A | 451 | 21.853 | -3.449 | 5.369 | 1.00 | 22.20 |
| 35 | ATOM | 1156 | CA | ILE | A | 451 | 21.385 | -3.741 | 6.726 | 1.00 | 22.82 |
| | ATOM | 1157 | CB | ILE | A | 451 | 21.452 | -2.476 | 7.616 | 1.00 | 19.62 |
| | ATOM | 1158 | CG2 | ILE | A | 451 | 20.593 | -2.658 | 8.886 | 1.00 | 21.11 |
| | ATOM | 1159 | CG1 | ILE | A | 451 | 22.909 | -2.210 | 7.999 | 1.00 | 22.20 |
| | ATOM | 1160 | CD1 | ILE | A | 451 | 23.115 | -0.960 | 8.850 | 1.00 | 24.48 |
| 40 | ATOM | 1161 | C | ILE | A | 451 | 19.952 | -4.250 | 6.662 | 1.00 | 21.82 |
| | ATOM | 1162 | O | ILE | A | 451 | 19.575 | -5.184 | 7.369 | 1.00 | 21.72 |
| | ATOM | 1163 | N | ILE | A | 452 | 19.152 | -3.642 | 5.795 | 1.00 | 20.18 |
| | ATOM | 1164 | CA | ILE | A | 452 | 17.763 | -4.058 | 5.649 | 1.00 | 18.13 |
| | ATOM | 1165 | CB | ILE | A | 452 | 17.024 | -3.145 | 4.627 | 1.00 | 19.72 |
| | ATOM | 1166 | CG2 | ILE | A | 452 | 15.720 | -3.792 | 4.169 | 1.00 | 18.99 |
| 45 | ATOM | 1167 | CG1 | ILE | A | 452 | 16.725 | -1.788 | 5.282 | 1.00 | 18.33 |
| | ATOM | 1168 | CD1 | ILE | A | 452 | 16.284 | -0.707 | 4.306 | 1.00 | 23.25 |
| | ATOM | 1169 | C | ILE | A | 452 | 17.725 | -5.517 | 5.191 | 1.00 | 19.50 |
| | ATOM | 1170 | O | ILE | A | 452 | 16.980 | -6.340 | 5.737 | 1.00 | 17.60 |
| 50 | ATOM | 1171 | N | LEU | A | 453 | 18.555 | -5.844 | 4.209 | 1.00 | 19.23 |
| | ATOM | 1172 | CA | LEU | A | 453 | 18.589 | -7.205 | 3.679 | 1.00 | 21.60 |
| | ATOM | 1173 | CB | LEU | A | 453 | 19.624 | -7.316 | 2.554 | 1.00 | 21.50 |
| | ATOM | 1174 | CG | LEU | A | 453 | 19.835 | -8.729 | 1.989 | 1.00 | 25.06 |
| | ATOM | 1175 | CD1 | LEU | A | 453 | 18.550 | -9.250 | 1.364 | 1.00 | 25.27 |
| | ATOM | 1176 | CD2 | LEU | A | 453 | 20.948 | -8.694 | 0.953 | 1.00 | 24.73 |
| 55 | ATOM | 1177 | C | LEU | A | 453 | 18.906 | -8.245 | 4.746 | 1.00 | 19.41 |
| | ATOM | 1178 | O | LEU | A | 453 | 18.198 | -9.241 | 4.891 | 1.00 | 20.75 |
| | ATOM | 1179 | N | LEU | A | 454 | 19.966 | -7.997 | 5.499 | 1.00 | 21.35 |
| | ATOM | 1180 | CA | LEU | A | 454 | 20.410 | -8.925 | 6.530 | 1.00 | 23.67 |
| 60 | ATOM | 1181 | CB | LEU | A | 454 | 21.870 | -8.625 | 6.878 | 1.00 | 20.69 |
| | ATOM | 1182 | CG | LEU | A | 454 | 22.816 | -8.584 | 5.673 | 1.00 | 24.92 |
| | ATOM | 1183 | CD1 | LEU | A | 454 | 24.222 | -8.268 | 6.132 | 1.00 | 24.27 |

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 1184 | CD2 | LEU | A | 454 | 22.785 | -9.913 | 4.952 | 1.00 | 22.84 |
| | ATOM | 1185 | C | LEU | A | 454 | 19.572 | -8.945 | 7.807 | 1.00 | 26.06 |
| | ATOM | 1186 | O | LEU | A | 454 | 19.413 | -9.997 | 8.438 | 1.00 | 27.44 |
| | ATOM | 1187 | N | ASN | A | 455 | 19.011 | -7.795 | 8.167 | 1.00 | 25.01 |
| | ATOM | 1188 | CA | ASN | A | 455 | 18.240 | -7.681 | 9.400 | 1.00 | 26.10 |
| 10 | ATOM | 1189 | CB | ASN | A | 455 | 18.439 | -6.295 | 10.002 | 1.00 | 22.67 |
| | ATOM | 1190 | CG | ASN | A | 455 | 17.627 | -6.109 | 11.264 | 1.00 | 26.67 |
| | ATOM | 1191 | OD1 | ASN | A | 455 | 17.899 | -6.751 | 12.270 | 1.00 | 25.16 |
| | ATOM | 1192 | ND2 | ASN | A | 455 | 16.615 | -5.246 | 11.212 | 1.00 | 20.73 |
| | ATOM | 1193 | C | ASN | A | 455 | 16.739 | -7.957 | 9.418 | 1.00 | 25.78 |
| 15 | ATOM | 1194 | O | ASN | A | 455 | 16.230 | -8.516 | 10.380 | 1.00 | 29.22 |
| | ATOM | 1195 | N | SER | A | 456 | 16.027 | -7.549 | 8.381 | 1.00 | 28.51 |
| | ATOM | 1196 | CA | SER | A | 456 | 14.578 | -7.704 | 8.371 | 1.00 | 32.52 |
| | ATOM | 1197 | CB | SER | A | 456 | 14.019 | -7.213 | 7.033 | 1.00 | 35.98 |
| | ATOM | 1198 | OG | SER | A | 456 | 14.266 | -5.818 | 6.897 | 1.00 | 30.88 |
| 20 | ATOM | 1199 | C | SER | A | 456 | 14.033 | -9.086 | 8.711 | 1.00 | 33.00 |
| | ATOM | 1200 | O | SER | A | 456 | 13.112 | -9.202 | 9.523 | 1.00 | 33.07 |
| | ATOM | 1201 | N | GLY | A | 457 | 14.597 | -10.130 | 8.117 | 1.00 | 28.40 |
| | ATOM | 1202 | CA | GLY | A | 457 | 14.115 | -11.464 | 8.413 | 1.00 | 36.28 |
| | ATOM | 1203 | C | GLY | A | 457 | 15.055 | -12.289 | 9.277 | 1.00 | 40.41 |
| 25 | ATOM | 1204 | O | GLY | A | 457 | 14.831 | -13.486 | 9.456 | 1.00 | 38.20 |
| | ATOM | 1205 | N | VAL | A | 458 | 16.095 | -11.657 | 9.820 | 1.00 | 44.13 |
| | ATOM | 1206 | CA | VAL | A | 458 | 17.079 | -12.356 | 10.647 | 1.00 | 51.09 |
| | ATOM | 1207 | CB | VAL | A | 458 | 18.214 | -11.399 | 11.095 | 1.00 | 51.06 |
| | ATOM | 1208 | CG1 | VAL | A | 458 | 17.688 | -10.390 | 12.104 | 1.00 | 51.75 |
| 30 | ATOM | 1209 | CG2 | VAL | A | 458 | 19.365 | -12.199 | 11.692 | 1.00 | 50.65 |
| | ATOM | 1210 | C | VAL | A | 458 | 16.513 | -13.060 | 11.885 | 1.00 | 57.26 |
| | ATOM | 1211 | O | VAL | A | 458 | 17.085 | -14.045 | 12.356 | 1.00 | 58.77 |
| | ATOM | 1212 | N | TYR | A | 459 | 15.401 | -12.560 | 12.416 | 1.00 | 62.31 |
| | ATOM | 1213 | CA | TYR | A | 459 | 14.793 | -13.177 | 13.592 | 1.00 | 68.49 |
| 35 | ATOM | 1214 | CB | TYR | A | 459 | 14.293 | -12.100 | 14.560 | 1.00 | 70.46 |
| | ATOM | 1215 | CG | TYR | A | 459 | 15.396 | -11.196 | 15.069 | 1.00 | 71.73 |
| | ATOM | 1216 | CD1 | TYR | A | 459 | 15.127 | -9.888 | 15.462 | 1.00 | 71.93 |
| | ATOM | 1217 | CE1 | TYR | A | 459 | 16.147 | -9.045 | 15.898 | 1.00 | 72.60 |
| | ATOM | 1218 | CD2 | TYR | A | 459 | 16.716 | -11.644 | 15.128 | 1.00 | 72.77 |
| 40 | ATOM | 1219 | CE2 | TYR | A | 459 | 17.741 | -10.812 | 15.560 | 1.00 | 73.55 |
| | ATOM | 1220 | CZ | TYR | A | 459 | 17.450 | -9.514 | 15.941 | 1.00 | 72.93 |
| | ATOM | 1221 | OH | TYR | A | 459 | 18.467 | -8.687 | 16.351 | 1.00 | 74.56 |
| | ATOM | 1222 | C | TYR | A | 459 | 13.649 | -14.097 | 13.187 | 1.00 | 71.86 |
| | ATOM | 1223 | O | TYR | A | 459 | 13.380 | -15.099 | 13.852 | 1.00 | 73.11 |
| 45 | ATOM | 1224 | N | THR | A | 460 | 12.981 | -13.756 | 12.090 | 1.00 | 74.84 |
| | ATOM | 1225 | CA | THR | A | 460 | 11.881 | -14.567 | 11.589 | 1.00 | 77.66 |
| | ATOM | 1226 | CB | THR | A | 460 | 11.246 | -13.900 | 10.373 | 1.00 | 76.69 |
| | ATOM | 1227 | C | THR | A | 460 | 12.436 | -15.938 | 11.212 | 1.00 | 80.26 |
| | ATOM | 1228 | O | THR | A | 460 | 11.684 | -16.866 | 10.912 | 1.00 | 80.82 |
| 50 | ATOM | 1229 | N | PHE | A | 461 | 13.762 | -16.051 | 11.231 | 1.00 | 82.69 |
| | ATOM | 1230 | CA | PHE | A | 461 | 14.440 | -17.299 | 10.905 | 1.00 | 85.63 |
| | ATOM | 1231 | CB | PHE | A | 461 | 15.920 | -17.034 | 10.630 | 1.00 | 85.47 |
| | ATOM | 1232 | C | PHE | A | 461 | 14.284 | -18.288 | 12.059 | 1.00 | 87.52 |
| | ATOM | 1233 | O | PHE | A | 461 | 14.493 | -17.940 | 13.224 | 1.00 | 86.53 |
| 55 | ATOM | 1234 | N | LEU | A | 462 | 13.914 | -19.520 | 11.724 | 1.00 | 89.49 |
| | ATOM | 1235 | CA | LEU | A | 462 | 13.711 | -20.568 | 12.718 | 1.00 | 91.34 |
| | ATOM | 1236 | CB | LEU | A | 462 | 12.961 | -21.741 | 12.087 | 1.00 | 91.23 |
| | ATOM | 1237 | C | LEU | A | 462 | 15.016 | -21.060 | 13.340 | 1.00 | 92.05 |
| | ATOM | 1238 | O | LEU | A | 462 | 16.042 | -21.165 | 12.664 | 1.00 | 91.91 |
| 60 | ATOM | 1239 | N | SER | A | 463 | 14.966 | -21.357 | 14.635 | 1.00 | 92.53 |
| | ATOM | 1240 | CA | SER | A | 463 | 16.131 | -21.855 | 15.358 | 1.00 | 92.96 |

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 1241 | CB | SER | A | 463 | 16.033 | -21.483 | 16.833 | 1.00 | 91.67 |
| | ATOM | 1242 | C | SER | A | 463 | 16.189 | -23.371 | 15.200 | 1.00 | 93.39 |
| | ATOM | 1243 | O | SER | A | 463 | 15.156 | -24.034 | 15.102 | 1.00 | 93.44 |
| | ATOM | 1244 | N | SER | A | 464 | 17.399 | -23.917 | 15.167 | 1.00 | 93.82 |
| | ATOM | 1245 | CA | SER | A | 464 | 17.577 | -25.355 | 15.015 | 1.00 | 93.85 |
| 10 | ATOM | 1246 | CB | SER | A | 464 | 17.284 | -25.769 | 13.577 | 1.00 | 93.74 |
| | ATOM | 1247 | C | SER | A | 464 | 18.997 | -25.743 | 15.396 | 1.00 | 93.96 |
| | ATOM | 1248 | O | SER | A | 464 | 19.815 | -26.074 | 14.535 | 1.00 | 93.65 |
| | ATOM | 1249 | N | THR | A | 465 | 19.279 | -25.699 | 16.694 | 1.00 | 93.91 |
| | ATOM | 1250 | CA | THR | A | 465 | 20.600 | -26.036 | 17.212 | 1.00 | 93.79 |
| 15 | ATOM | 1251 | CB | THR | A | 465 | 20.952 | -27.483 | 16.863 | 1.00 | 93.38 |
| | ATOM | 1252 | C | THR | A | 465 | 21.640 | -25.085 | 16.634 | 1.00 | 93.27 |
| | ATOM | 1253 | O | THR | A | 465 | 21.302 | -24.017 | 16.121 | 1.00 | 93.03 |
| | ATOM | 1254 | N | LEU | A | 466 | 22.907 | -25.479 | 16.723 | 1.00 | 93.26 |
| | ATOM | 1255 | CA | LEU | A | 466 | 23.999 | -24.665 | 16.207 | 1.00 | 92.34 |
| 20 | ATOM | 1256 | CB | LEU | A | 466 | 25.335 | -25.338 | 16.498 | 1.00 | 91.59 |
| | ATOM | 1257 | C | LEU | A | 466 | 23.829 | -24.461 | 14.706 | 1.00 | 92.18 |
| | ATOM | 1258 | O | LEU | A | 466 | 24.411 | -23.545 | 14.125 | 1.00 | 92.67 |
| | ATOM | 1259 | N | LYS | A | 467 | 23.028 | -25.323 | 14.086 | 1.00 | 91.28 |
| | ATOM | 1260 | CA | LYS | A | 467 | 22.772 | -25.238 | 12.653 | 1.00 | 90.02 |
| 25 | ATOM | 1261 | CB | LYS | A | 467 | 21.740 | -26.287 | 12.240 | 1.00 | 89.93 |
| | ATOM | 1262 | C | LYS | A | 467 | 22.269 | -23.841 | 12.308 | 1.00 | 88.35 |
| | ATOM | 1263 | O | LYS | A | 467 | 23.032 | -22.990 | 11.849 | 1.00 | 88.50 |
| | ATOM | 1264 | N | SER | A | 468 | 20.981 | -23.610 | 12.536 | 1.00 | 86.02 |
| | ATOM | 1265 | CA | SER | A | 468 | 20.384 | -22.315 | 12.252 | 1.00 | 84.10 |
| 30 | ATOM | 1266 | CB | SER | A | 468 | 18.901 | -22.333 | 12.620 | 1.00 | 84.08 |
| | ATOM | 1267 | OG | SER | A | 468 | 18.229 | -23.378 | 11.937 | 1.00 | 83.03 |
| | ATOM | 1268 | C | SER | A | 468 | 21.109 | -21.230 | 13.040 | 1.00 | 83.39 |
| | ATOM | 1269 | O | SER | A | 468 | 21.264 | -20.105 | 12.565 | 1.00 | 83.48 |
| | ATOM | 1270 | N | LEU | A | 469 | 21.558 | -21.579 | 14.242 | 1.00 | 82.04 |
| 35 | ATOM | 1271 | CA | LEU | A | 469 | 22.276 | -20.640 | 15.098 | 1.00 | 80.28 |
| | ATOM | 1272 | CB | LEU | A | 469 | 22.595 | -21.294 | 16.436 | 1.00 | 79.81 |
| | ATOM | 1273 | C | LEU | A | 469 | 23.564 | -20.174 | 14.419 | 1.00 | 79.18 |
| | ATOM | 1274 | O | LEU | A | 469 | 24.111 | -19.122 | 14.756 | 1.00 | 78.61 |
| | ATOM | 1275 | N | GLU | A | 470 | 24.044 | -20.969 | 13.466 | 1.00 | 76.69 |
| 40 | ATOM | 1276 | CA | GLU | A | 470 | 25.256 | -20.638 | 12.726 | 1.00 | 74.84 |
| | ATOM | 1277 | CB | GLU | A | 470 | 25.803 | -21.880 | 12.032 | 1.00 | 74.12 |
| | ATOM | 1278 | C | GLU | A | 470 | 24.920 | -19.565 | 11.697 | 1.00 | 73.77 |
| | ATOM | 1279 | O | GLU | A | 470 | 25.617 | -18.556 | 11.581 | 1.00 | 72.94 |
| | ATOM | 1280 | N | GLU | A | 471 | 23.842 | -19.792 | 10.953 | 1.00 | 72.08 |
| 45 | ATOM | 1281 | CA | GLU | A | 471 | 23.396 | -18.842 | 9.945 | 1.00 | 70.05 |
| | ATOM | 1282 | CB | GLU | A | 471 | 22.461 | -19.526 | 8.944 | 1.00 | 71.52 |
| | ATOM | 1283 | CG | GLU | A | 471 | 23.150 | -19.976 | 7.668 | 1.00 | 72.90 |
| | ATOM | 1284 | CD | GLU | A | 471 | 24.512 | -20.586 | 7.932 | 1.00 | 74.01 |
| | ATOM | 1285 | OE1 | GLU | A | 471 | 25.469 | -20.258 | 7.198 | 1.00 | 74.22 |
| 50 | ATOM | 1286 | OE2 | GLU | A | 471 | 24.626 | -21.395 | 8.878 | 1.00 | 75.18 |
| | ATOM | 1287 | C | GLU | A | 471 | 22.667 | -17.692 | 10.630 | 1.00 | 67.33 |
| | ATOM | 1288 | O | GLU | A | 471 | 21.685 | -17.165 | 10.107 | 1.00 | 67.77 |
| | ATOM | 1289 | N | LYS | A | 472 | 23.152 | -17.319 | 11.811 | 1.00 | 62.63 |
| | ATOM | 1290 | CA | LYS | A | 472 | 22.564 | -16.229 | 12.578 | 1.00 | 57.41 |
| 55 | ATOM | 1291 | CB | LYS | A | 472 | 21.697 | -16.777 | 13.713 | 1.00 | 58.74 |
| | ATOM | 1292 | CG | LYS | A | 472 | 20.683 | -15.776 | 14.243 | 1.00 | 60.32 |
| | ATOM | 1293 | CD | LYS | A | 472 | 19.271 | -16.342 | 14.219 | 1.00 | 60.73 |
| | ATOM | 1294 | CE | LYS | A | 472 | 18.485 | -15.909 | 15.449 | 1.00 | 61.78 |
| | ATOM | 1295 | NZ | LYS | A | 472 | 19.352 | -15.788 | 16.658 | 1.00 | 60.09 |
| 60 | ATOM | 1296 | C | LYS | A | 472 | 23.662 | -15.339 | 13.150 | 1.00 | 53.42 |
| | ATOM | 1297 | O | LYS | A | 472 | 23.631 | -14.120 | 12.978 | 1.00 | 50.87 |

| | | | | | | | | | | | |
|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 1298 | N | ASP | A | 473 | 24.628 | -15.949 | 13.830 | 1.00 | 47.52 |
| | ATOM | 1299 | CA | ASP | A | 473 | 25.732 | -15.194 | 14.405 | 1.00 | 45.55 |
| | ATOM | 1300 | CB | ASP | A | 473 | 26.613 | -16.094 | 15.269 | 1.00 | 50.48 |
| | ATOM | 1301 | CG | ASP | A | 473 | 26.380 | -15.885 | 16.749 | 1.00 | 55.50 |
| | ATOM | 1302 | OD1 | ASP | A | 473 | 25.272 | -15.436 | 17.118 | 1.00 | 58.06 |
| 10 | ATOM | 1303 | OD2 | ASP | A | 473 | 27.304 | -16.170 | 17.541 | 1.00 | 59.81 |
| | ATOM | 1304 | C | ASP | A | 473 | 26.557 | -14.611 | 13.269 | 1.00 | 42.62 |
| | ATOM | 1305 | O | ASP | A | 473 | 27.087 | -13.506 | 13.373 | 1.00 | 42.10 |
| | ATOM | 1306 | N | HIS | A | 474 | 26.663 | -15.364 | 12.180 | 1.00 | 38.05 |
| | ATOM | 1307 | CA | HIS | A | 474 | 27.416 | -14.904 | 11.026 | 1.00 | 37.25 |
| 15 | ATOM | 1308 | CB | HIS | A | 474 | 27.429 | -15.978 | 9.941 | 1.00 | 35.07 |
| | ATOM | 1309 | CG | HIS | A | 474 | 28.036 | -15.523 | 8.653 | 1.00 | 37.36 |
| | ATOM | 1310 | CD2 | HIS | A | 474 | 29.292 | -15.113 | 8.355 | 1.00 | 38.86 |
| | ATOM | 1311 | ND1 | HIS | A | 474 | 27.322 | -15.452 | 7.476 | 1.00 | 41.31 |
| | ATOM | 1312 | CE1 | HIS | A | 474 | 28.110 | -15.020 | 6.509 | 1.00 | 40.86 |
| 20 | ATOM | 1313 | NE2 | HIS | A | 474 | 29.311 | -14.807 | 7.016 | 1.00 | 44.49 |
| | ATOM | 1314 | C | HIS | A | 474 | 26.749 | -13.640 | 10.493 | 1.00 | 36.68 |
| | ATOM | 1315 | O | HIS | A | 474 | 27.417 | -12.676 | 10.132 | 1.00 | 36.48 |
| | ATOM | 1316 | N | ILE | A | 475 | 25.422 | -13.652 | 10.447 | 1.00 | 35.93 |
| | ATOM | 1317 | CA | ILE | A | 475 | 24.683 | -12.499 | 9.963 | 1.00 | 36.21 |
| 25 | ATOM | 1318 | CB | ILE | A | 475 | 23.174 | -12.797 | 9.868 | 1.00 | 36.31 |
| | ATOM | 1319 | CG2 | ILE | A | 475 | 22.411 | -11.527 | 9.513 | 1.00 | 38.19 |
| | ATOM | 1320 | CG1 | ILE | A | 475 | 22.922 | -13.874 | 8.813 | 1.00 | 36.97 |
| | ATOM | 1321 | CD1 | ILE | A | 475 | 21.528 | -14.454 | 8.869 | 1.00 | 35.59 |
| | ATOM | 1322 | C | ILE | A | 475 | 24.893 | -11.322 | 10.907 | 1.00 | 35.34 |
| 30 | ATOM | 1323 | O | ILE | A | 475 | 25.092 | -10.189 | 10.471 | 1.00 | 33.20 |
| | ATOM | 1324 | N | HIS | A | 476 | 24.857 | -11.596 | 12.206 | 1.00 | 35.95 |
| | ATOM | 1325 | CA | HIS | A | 476 | 25.031 | -10.540 | 13.193 | 1.00 | 35.06 |
| | ATOM | 1326 | CB | HIS | A | 476 | 24.681 | -11.062 | 14.585 | 1.00 | 37.30 |
| | ATOM | 1327 | CG | HIS | A | 476 | 23.210 | -11.068 | 14.860 | 1.00 | 43.06 |
| 35 | ATOM | 1328 | CD2 | HIS | A | 476 | 22.329 | -10.051 | 15.017 | 1.00 | 43.93 |
| | ATOM | 1329 | ND1 | HIS | A | 476 | 22.476 | -12.230 | 14.968 | 1.00 | 45.60 |
| | ATOM | 1330 | CE1 | HIS | A | 476 | 21.207 | -11.928 | 15.177 | 1.00 | 47.56 |
| | ATOM | 1331 | NE2 | HIS | A | 476 | 21.091 | -10.613 | 15.211 | 1.00 | 46.21 |
| | ATOM | 1332 | C | HIS | A | 476 | 26.438 | -9.966 | 13.170 | 1.00 | 35.40 |
| 40 | ATOM | 1333 | O | HIS | A | 476 | 26.634 | -8.774 | 13.415 | 1.00 | 35.45 |
| | ATOM | 1334 | N | ARG | A | 477 | 27.420 | -10.805 | 12.862 | 1.00 | 34.07 |
| | ATOM | 1335 | CA | ARG | A | 477 | 28.796 | -10.331 | 12.795 | 1.00 | 34.18 |
| | ATOM | 1336 | CB | ARG | A | 477 | 29.757 | -11.506 | 12.605 | 1.00 | 41.04 |
| | ATOM | 1337 | CG | ARG | A | 477 | 29.800 | -12.459 | 13.788 | 1.00 | 47.61 |
| 45 | ATOM | 1338 | CD | ARG | A | 477 | 30.782 | -13.599 | 13.557 | 1.00 | 55.67 |
| | ATOM | 1339 | NE | ARG | A | 477 | 31.780 | -13.675 | 14.622 | 1.00 | 60.17 |
| | ATOM | 1340 | CZ | ARG | A | 477 | 32.780 | -12.811 | 14.770 | 1.00 | 61.98 |
| | ATOM | 1341 | NH1 | ARG | A | 477 | 32.918 | -11.803 | 13.918 | 1.00 | 64.29 |
| | ATOM | 1342 | NH2 | ARG | A | 477 | 33.643 | -12.955 | 15.766 | 1.00 | 62.79 |
| 50 | ATOM | 1343 | C | ARG | A | 477 | 28.906 | -9.361 | 11.621 | 1.00 | 30.77 |
| | ATOM | 1344 | O | ARG | A | 477 | 29.462 | -8.268 | 11.753 | 1.00 | 33.59 |
| | ATOM | 1345 | N | VAL | A | 478 | 28.369 | -9.766 | 10.475 | 1.00 | 27.65 |
| | ATOM | 1346 | CA | VAL | A | 478 | 28.389 | -8.930 | 9.280 | 1.00 | 27.07 |
| | ATOM | 1347 | CB | VAL | A | 478 | 27.658 | -9.605 | 8.100 | 1.00 | 28.00 |
| 55 | ATOM | 1348 | CG1 | VAL | A | 478 | 27.672 | -8.678 | 6.890 | 1.00 | 25.83 |
| | ATOM | 1349 | CG2 | VAL | A | 478 | 28.319 | -10.933 | 7.761 | 1.00 | 31.66 |
| | ATOM | 1350 | C | VAL | A | 478 | 27.689 | -7.610 | 9.584 | 1.00 | 26.92 |
| | ATOM | 1351 | O | VAL | A | 478 | 28.216 | -6.536 | 9.294 | 1.00 | 26.97 |
| | ATOM | 1352 | N | LEU | A | 479 | 26.499 | -7.702 | 10.171 | 1.00 | 25.74 |
| 60 | ATOM | 1353 | CA | LEU | A | 479 | 25.727 | -6.516 | 10.530 | 1.00 | 27.97 |
| | ATOM | 1354 | CB | LEU | A | 479 | 24.474 | -6.912 | 11.324 | 1.00 | 25.55 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1355 | CG | LEU | A | 479 | 23.211 | -7.229 | 10.517 | 1.00 | 29.01 |
| | ATOM | 1356 | CD1 | LEU | A | 479 | 22.056 | -7.503 | 11.481 | 1.00 | 27.05 |
| | ATOM | 1357 | CD2 | LEU | A | 479 | 22.864 | -6.063 | 9.584 | 1.00 | 24.92 |
| | ATOM | 1358 | C | LEU | A | 479 | 26.592 | -5.582 | 11.369 | 1.00 | 25.39 |
| | ATOM | 1359 | O | LEU | A | 479 | 26.595 | -4.370 | 11.158 | 1.00 | 27.39 |
| 10 | ATOM | 1360 | N | ASP | A | 480 | 27.324 | -6.158 | 12.320 | 1.00 | 26.04 |
| | ATOM | 1361 | CA | ASP | A | 480 | 28.206 | -5.388 | 13.193 | 1.00 | 27.32 |
| | ATOM | 1362 | CB | ASP | A | 480 | 28.878 | -6.305 | 14.222 | 1.00 | 26.67 |
| | ATOM | 1363 | CG | ASP | A | 480 | 27.990 | -6.602 | 15.417 | 1.00 | 31.02 |
| | ATOM | 1364 | OD1 | ASP | A | 480 | 28.355 | -7.505 | 16.198 | 1.00 | 31.50 |
| 15 | ATOM | 1365 | OD2 | ASP | A | 480 | 26.935 | -5.944 | 15.580 | 1.00 | 32.21 |
| | ATOM | 1366 | C | ASP | A | 480 | 29.283 | -4.699 | 12.361 | 1.00 | 25.59 |
| | ATOM | 1367 | O | ASP | A | 480 | 29.672 | -3.562 | 12.636 | 1.00 | 27.15 |
| | ATOM | 1368 | N | LYS | A | 481 | 29.767 | -5.394 | 11.340 | 1.00 | 25.17 |
| | ATOM | 1369 | CA | LYS | A | 481 | 30.794 | -4.830 | 10.477 | 1.00 | 24.93 |
| 20 | ATOM | 1370 | CB | LYS | A | 481 | 31.306 | -5.890 | 9.512 | 1.00 | 28.42 |
| | ATOM | 1371 | CG | LYS | A | 481 | 32.158 | -6.953 | 10.188 | 1.00 | 35.59 |
| | ATOM | 1372 | CD | LYS | A | 481 | 32.894 | -7.799 | 9.157 | 1.00 | 41.21 |
| | ATOM | 1373 | CE | LYS | A | 481 | 33.883 | -6.963 | 8.350 | 1.00 | 41.48 |
| | ATOM | 1374 | NZ | LYS | A | 481 | 34.954 | -6.388 | 9.215 | 1.00 | 43.22 |
| 25 | ATOM | 1375 | C | LYS | A | 481 | 30.260 | -3.635 | 9.696 | 1.00 | 26.12 |
| | ATOM | 1376 | O | LYS | A | 481 | 30.979 | -2.657 | 9.463 | 1.00 | 23.73 |
| | ATOM | 1377 | N | ILE | A | 482 | 28.996 | -3.705 | 9.291 | 1.00 | 25.44 |
| | ATOM | 1378 | CA | ILE | A | 482 | 28.421 | -2.598 | 8.545 | 1.00 | 27.69 |
| | ATOM | 1379 | CB | ILE | A | 482 | 27.066 | -2.983 | 7.915 | 1.00 | 27.59 |
| 30 | ATOM | 1380 | CG2 | ILE | A | 482 | 26.470 | -1.788 | 7.183 | 1.00 | 25.97 |
| | ATOM | 1381 | CG1 | ILE | A | 482 | 27.274 | -4.131 | 6.922 | 1.00 | 23.80 |
| | ATOM | 1382 | CD1 | ILE | A | 482 | 26.000 | -4.838 | 6.533 | 1.00 | 21.30 |
| | ATOM | 1383 | C | ILE | A | 482 | 28.253 | -1.408 | 9.481 | 1.00 | 27.33 |
| | ATOM | 1384 | O | ILE | A | 482 | 28.312 | -0.256 | 9.045 | 1.00 | 28.55 |
| 35 | ATOM | 1385 | N | THR | A | 483 | 28.046 | -1.690 | 10.768 | 1.00 | 25.03 |
| | ATOM | 1386 | CA | THR | A | 483 | 27.905 | -0.632 | 11.760 | 1.00 | 23.62 |
| | ATOM | 1387 | CB | THR | A | 483 | 27.535 | -1.192 | 13.154 | 1.00 | 22.18 |
| | ATOM | 1388 | OG1 | THR | A | 483 | 26.181 | -1.658 | 13.133 | 1.00 | 25.39 |
| | ATOM | 1389 | CG2 | THR | A | 483 | 27.673 | -0.111 | 14.226 | 1.00 | 25.84 |
| 40 | ATOM | 1390 | C | THR | A | 483 | 29.257 | 0.074 | 11.858 | 1.00 | 23.04 |
| | ATOM | 1391 | O | THR | A | 483 | 29.331 | 1.306 | 11.846 | 1.00 | 23.55 |
| | ATOM | 1392 | N | ASP | A | 484 | 30.324 | -0.714 | 11.960 | 1.00 | 22.24 |
| | ATOM | 1393 | CA | ASP | A | 484 | 31.674 | -0.152 | 12.039 | 1.00 | 25.48 |
| | ATOM | 1394 | CB | ASP | A | 484 | 32.718 | -1.273 | 12.107 | 1.00 | 26.88 |
| 45 | ATOM | 1395 | CG | ASP | A | 484 | 32.629 | -2.083 | 13.394 | 1.00 | 32.52 |
| | ATOM | 1396 | OD1 | ASP | A | 484 | 32.002 | -1.608 | 14.366 | 1.00 | 33.68 |
| | ATOM | 1397 | OD2 | ASP | A | 484 | 33.185 | -3.198 | 13.434 | 1.00 | 34.63 |
| | ATOM | 1398 | C | ASP | A | 484 | 31.930 | 0.715 | 10.807 | 1.00 | 25.16 |
| | ATOM | 1399 | O | ASP | A | 484 | 32.481 | 1.812 | 10.905 | 1.00 | 26.05 |
| 50 | ATOM | 1400 | N | THR | A | 485 | 31.505 | 0.226 | 9.645 | 1.00 | 28.96 |
| | ATOM | 1401 | CA | THR | A | 485 | 31.689 | 0.960 | 8.394 | 1.00 | 26.63 |
| | ATOM | 1402 | CB | THR | A | 485 | 31.124 | 0.166 | 7.197 | 1.00 | 26.12 |
| | ATOM | 1403 | OG1 | THR | A | 485 | 31.753 | -1.123 | 7.132 | 1.00 | 24.30 |
| | ATOM | 1404 | CG2 | THR | A | 485 | 31.381 | 0.907 | 5.898 | 1.00 | 23.31 |
| 55 | ATOM | 1405 | C | THR | A | 485 | 30.994 | 2.318 | 8.468 | 1.00 | 28.90 |
| | ATOM | 1406 | O | THR | A | 485 | 31.583 | 3.354 | 8.137 | 1.00 | 27.26 |
| | ATOM | 1407 | N | LEU | A | 486 | 29.743 | 2.310 | 8.915 | 1.00 | 24.76 |
| | ATOM | 1408 | CA | LEU | A | 486 | 28.973 | 3.537 | 9.027 | 1.00 | 26.19 |
| | ATOM | 1409 | CB | LEU | A | 486 | 27.567 | 3.233 | 9.547 | 1.00 | 27.27 |
| 60 | ATOM | 1410 | CG | LEU | A | 486 | 26.508 | 2.921 | 8.486 | 1.00 | 23.50 |
| | ATOM | 1411 | CD1 | LEU | A | 486 | 25.210 | 2.550 | 9.183 | 1.00 | 22.03 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1412 | CD2 | LEU | A | 486 | 26.309 | 4.128 | 7.577 | 1.00 | 21.35 |
| | ATOM | 1413 | C | LEU | A | 486 | 29.662 | 4.519 | 9.960 | 1.00 | 27.36 |
| | ATOM | 1414 | O | LEU | A | 486 | 29.745 | 5.710 | 9.669 | 1.00 | 25.87 |
| | ATOM | 1415 | N | ILE | A | 487 | 30.151 | 4.015 | 11.088 | 1.00 | 27.88 |
| | ATOM | 1416 | CA | ILE | A | 487 | 30.843 | 4.857 | 12.055 | 1.00 | 28.40 |
| 10 | ATOM | 1417 | CB | ILE | A | 487 | 31.203 | 4.054 | 13.332 | 1.00 | 26.74 |
| | ATOM | 1418 | CG2 | ILE | A | 487 | 32.255 | 4.803 | 14.154 | 1.00 | 27.54 |
| | ATOM | 1419 | CG1 | ILE | A | 487 | 29.937 | 3.813 | 14.163 | 1.00 | 25.93 |
| | ATOM | 1420 | CD1 | ILE | A | 487 | 29.237 | 5.088 | 14.624 | 1.00 | 23.42 |
| | ATOM | 1421 | C | ILE | A | 487 | 32.125 | 5.393 | 11.412 | 1.00 | 28.89 |
| 15 | ATOM | 1422 | O | ILE | A | 487 | 32.497 | 6.554 | 11.602 | 1.00 | 29.85 |
| | ATOM | 1423 | N | HIS | A | 488 | 32.791 | 4.533 | 10.649 | 1.00 | 29.71 |
| | ATOM | 1424 | CA | HIS | A | 488 | 34.031 | 4.898 | 9.967 | 1.00 | 34.12 |
| | ATOM | 1425 | CB | HIS | A | 488 | 34.585 | 3.691 | 9.207 | 1.00 | 36.61 |
| | ATOM | 1426 | CG | HIS | A | 488 | 35.799 | 3.997 | 8.385 | 1.00 | 42.74 |
| 20 | ATOM | 1427 | CD2 | HIS | A | 488 | 35.970 | 4.089 | 7.045 | 1.00 | 43.12 |
| | ATOM | 1428 | ND1 | HIS | A | 488 | 37.034 | 4.239 | 8.946 | 1.00 | 43.13 |
| | ATOM | 1429 | CE1 | HIS | A | 488 | 37.913 | 4.466 | 7.987 | 1.00 | 43.40 |
| | ATOM | 1430 | NE2 | HIS | A | 488 | 37.293 | 4.381 | 6.825 | 1.00 | 45.63 |
| | ATOM | 1431 | C | HIS | A | 488 | 33.799 | 6.051 | 8.998 | 1.00 | 32.74 |
| 25 | ATOM | 1432 | O | HIS | A | 488 | 34.577 | 7.004 | 8.955 | 1.00 | 31.06 |
| | ATOM | 1433 | N | LEU | A | 489 | 32.721 | 5.958 | 8.223 | 1.00 | 33.56 |
| | ATOM | 1434 | CA | LEU | A | 489 | 32.384 | 6.992 | 7.258 | 1.00 | 30.78 |
| | ATOM | 1435 | CB | LEU | A | 489 | 31.145 | 6.587 | 6.464 | 1.00 | 34.67 |
| | ATOM | 1436 | CG | LEU | A | 489 | 31.310 | 5.353 | 5.574 | 1.00 | 34.73 |
| 30 | ATOM | 1437 | CD1 | LEU | A | 489 | 29.945 | 4.856 | 5.125 | 1.00 | 33.21 |
| | ATOM | 1438 | CD2 | LEU | A | 489 | 32.183 | 5.701 | 4.378 | 1.00 | 35.92 |
| | ATOM | 1439 | C | LEU | A | 489 | 32.124 | 8.320 | 7.954 | 1.00 | 33.97 |
| | ATOM | 1440 | O | LEU | A | 489 | 32.587 | 9.365 | 7.507 | 1.00 | 33.22 |
| | ATOM | 1441 | N | MET | A | 490 | 31.387 | 8.274 | 9.058 | 1.00 | 31.33 |
| 35 | ATOM | 1442 | CA | MET | A | 490 | 31.056 | 9.482 | 9.801 | 1.00 | 30.61 |
| | ATOM | 1443 | CB | MET | A | 490 | 30.000 | 9.161 | 10.862 | 1.00 | 32.34 |
| | ATOM | 1444 | CG | MET | A | 490 | 28.607 | 8.940 | 10.289 | 1.00 | 30.71 |
| | ATOM | 1445 | SD | MET | A | 490 | 27.457 | 8.247 | 11.496 | 1.00 | 31.14 |
| | ATOM | 1446 | CE | MET | A | 490 | 26.321 | 7.408 | 10.418 | 1.00 | 30.36 |
| 40 | ATOM | 1447 | C | MET | A | 490 | 32.287 | 10.108 | 10.455 | 1.00 | 32.22 |
| | ATOM | 1448 | O | MET | A | 490 | 32.412 | 11.330 | 10.517 | 1.00 | 28.25 |
| | ATOM | 1449 | N | ALA | A | 491 | 33.184 | 9.262 | 10.949 | 1.00 | 33.81 |
| | ATOM | 1450 | CA | ALA | A | 491 | 34.407 | 9.730 | 11.585 | 1.00 | 39.92 |
| | ATOM | 1451 | CB | ALA | A | 491 | 35.168 | 8.554 | 12.185 | 1.00 | 37.22 |
| 45 | ATOM | 1452 | C | ALA | A | 491 | 35.275 | 10.445 | 10.550 | 1.00 | 42.68 |
| | ATOM | 1453 | O | ALA | A | 491 | 35.865 | 11.487 | 10.838 | 1.00 | 45.32 |
| | ATOM | 1454 | N | LYS | A | 492 | 35.339 | 9.876 | 9.347 | 1.00 | 44.39 |
| | ATOM | 1455 | CA | LYS | A | 492 | 36.122 | 10.440 | 8.248 | 1.00 | 44.80 |
| | ATOM | 1456 | CB | LYS | A | 492 | 36.136 | 9.477 | 7.052 | 1.00 | 46.96 |
| 50 | ATOM | 1457 | CG | LYS | A | 492 | 37.490 | 8.840 | 6.744 | 1.00 | 47.20 |
| | ATOM | 1458 | CD | LYS | A | 492 | 37.390 | 7.830 | 5.595 | 1.00 | 45.71 |
| | ATOM | 1459 | CE | LYS | A | 492 | 38.631 | 6.937 | 5.518 | 1.00 | 45.55 |
| | ATOM | 1460 | NZ | LYS | A | 492 | 38.357 | 5.577 | 4.948 | 1.00 | 36.28 |
| | ATOM | 1461 | C | LYS | A | 492 | 35.534 | 11.780 | 7.809 | 1.00 | 45.61 |
| 55 | ATOM | 1462 | O | LYS | A | 492 | 36.227 | 12.604 | 7.215 | 1.00 | 46.18 |
| | ATOM | 1463 | N | ALA | A | 493 | 34.254 | 11.992 | 8.100 | 1.00 | 43.75 |
| | ATOM | 1464 | CA | ALA | A | 493 | 33.590 | 13.238 | 7.728 | 1.00 | 42.42 |
| | ATOM | 1465 | CB | ALA | A | 493 | 32.097 | 13.001 | 7.528 | 1.00 | 40.92 |
| | ATOM | 1466 | C | ALA | A | 493 | 33.816 | 14.305 | 8.796 | 1.00 | 41.78 |
| 60 | ATOM | 1467 | O | ALA | A | 493 | 33.277 | 15.410 | 8.707 | 1.00 | 40.76 |
| | ATOM | 1468 | N | GLY | A | 494 | 34.604 | 13.960 | 9.811 | 1.00 | 41.01 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1469 | CA | GLY | A | 494 | 34.903 | 14.904 | 10.873 | 1.00 | 41.63 |
| | ATOM | 1470 | C | GLY | A | 494 | 33.857 | 15.060 | 11.965 | 1.00 | 41.18 |
| | ATOM | 1471 | O | GLY | A | 494 | 33.916 | 16.011 | 12.747 | 1.00 | 38.22 |
| | ATOM | 1472 | N | LEU | A | 495 | 32.905 | 14.138 | 12.043 | 1.00 | 39.53 |
| | ATOM | 1473 | CA | LEU | A | 495 | 31.876 | 14.248 | 13.068 | 1.00 | 38.91 |
| 10 | ATOM | 1474 | CB | LEU | A | 495 | 30.713 | 13.304 | 12.769 | 1.00 | 39.20 |
| | ATOM | 1475 | CG | LEU | A | 495 | 29.540 | 13.901 | 11.988 | 1.00 | 40.73 |
| | ATOM | 1476 | CD1 | LEU | A | 495 | 29.976 | 14.170 | 10.553 | 1.00 | 37.80 |
| | ATOM | 1477 | CD2 | LEU | A | 495 | 28.349 | 12.943 | 12.026 | 1.00 | 40.94 |
| | ATOM | 1478 | C | LEU | A | 495 | 32.461 | 13.923 | 14.431 | 1.00 | 36.01 |
| 15 | ATOM | 1479 | O | LEU | A | 495 | 33.347 | 13.074 | 14.544 | 1.00 | 34.85 |
| | ATOM | 1480 | N | THR | A | 496 | 31.979 | 14.604 | 15.459 | 1.00 | 37.52 |
| | ATOM | 1481 | CA | THR | A | 496 | 32.462 | 14.350 | 16.812 | 1.00 | 35.45 |
| | ATOM | 1482 | CB | THR | A | 496 | 31.925 | 15.375 | 17.829 | 1.00 | 37.55 |
| | ATOM | 1483 | OG1 | THR | A | 496 | 30.498 | 15.263 | 17.908 | 1.00 | 32.93 |
| 20 | ATOM | 1484 | CG2 | THR | A | 496 | 32.315 | 16.797 | 17.434 | 1.00 | 36.16 |
| | ATOM | 1485 | C | THR | A | 496 | 31.933 | 12.987 | 17.210 | 1.00 | 35.67 |
| | ATOM | 1486 | O | THR | A | 496 | 31.081 | 12.427 | 16.521 | 1.00 | 34.34 |
| | ATOM | 1487 | N | LEU | A | 497 | 32.429 | 12.452 | 18.319 | 1.00 | 34.88 |
| | ATOM | 1488 | CA | LEU | A | 497 | 31.965 | 11.151 | 18.786 | 1.00 | 35.67 |
| 25 | ATOM | 1489 | CB | LEU | A | 497 | 32.689 | 10.760 | 20.074 | 1.00 | 41.10 |
| | ATOM | 1490 | CG | LEU | A | 497 | 33.714 | 9.640 | 19.896 | 1.00 | 45.27 |
| | ATOM | 1491 | CD1 | LEU | A | 497 | 34.755 | 9.692 | 21.008 | 1.00 | 45.09 |
| | ATOM | 1492 | CD2 | LEU | A | 497 | 32.988 | 8.305 | 19.884 | 1.00 | 47.77 |
| | ATOM | 1493 | C | LEU | A | 497 | 30.455 | 11.198 | 19.026 | 1.00 | 33.72 |
| 30 | ATOM | 1494 | O | LEU | A | 497 | 29.712 | 10.350 | 18.534 | 1.00 | 33.20 |
| | ATOM | 1495 | N | GLN | A | 498 | 30.006 | 12.202 | 19.773 | 1.00 | 30.82 |
| | ATOM | 1496 | CA | GLN | A | 498 | 28.586 | 12.348 | 20.062 | 1.00 | 31.47 |
| | ATOM | 1497 | CB | GLN | A | 498 | 28.344 | 13.566 | 20.951 | 1.00 | 30.51 |
| | ATOM | 1498 | CG | GLN | A | 498 | 26.894 | 13.796 | 21.341 | 1.00 | 34.38 |
| 35 | ATOM | 1499 | CD | GLN | A | 498 | 26.712 | 15.130 | 22.015 | 1.00 | 38.60 |
| | ATOM | 1500 | OE1 | GLN | A | 498 | 27.363 | 16.112 | 21.686 | 1.00 | 42.92 |
| | ATOM | 1501 | NE2 | GLN | A | 498 | 25.809 | 15.176 | 23.008 | 1.00 | 40.02 |
| | ATOM | 1502 | C | GLN | A | 498 | 27.776 | 12.476 | 18.773 | 1.00 | 30.47 |
| | ATOM | 1503 | O | GLN | A | 498 | 26.682 | 11.927 | 18.665 | 1.00 | 30.85 |
| 40 | ATOM | 1504 | N | GLN | A | 499 | 28.311 | 13.196 | 17.793 | 1.00 | 29.52 |
| | ATOM | 1505 | CA | GLN | A | 499 | 27.603 | 13.362 | 16.524 | 1.00 | 30.24 |
| | ATOM | 1506 | CB | GLN | A | 499 | 28.292 | 14.420 | 15.661 | 1.00 | 30.20 |
| | ATOM | 1507 | CG | GLN | A | 499 | 28.135 | 15.840 | 16.191 | 1.00 | 31.60 |
| | ATOM | 1508 | CD | GLN | A | 499 | 28.930 | 16.849 | 15.389 | 1.00 | 31.61 |
| 45 | ATOM | 1509 | OE1 | GLN | A | 499 | 29.956 | 16.518 | 14.795 | 1.00 | 30.66 |
| | ATOM | 1510 | NE2 | GLN | A | 499 | 28.457 | 18.089 | 15.364 | 1.00 | 34.17 |
| | ATOM | 1511 | C | GLN | A | 499 | 27.529 | 12.047 | 15.753 | 1.00 | 29.40 |
| | ATOM | 1512 | O | GLN | A | 499 | 26.567 | 11.793 | 15.032 | 1.00 | 30.04 |
| | ATOM | 1513 | N | GLN | A | 500 | 28.550 | 11.214 | 15.903 | 1.00 | 25.67 |
| 50 | ATOM | 1514 | CA | GLN | A | 500 | 28.577 | 9.937 | 15.216 | 1.00 | 29.30 |
| | ATOM | 1515 | CB | GLN | A | 500 | 29.933 | 9.276 | 15.406 | 1.00 | 31.52 |
| | ATOM | 1516 | CG | GLN | A | 500 | 31.012 | 9.839 | 14.508 | 1.00 | 33.05 |
| | ATOM | 1517 | CD | GLN | A | 500 | 32.371 | 9.370 | 14.930 | 1.00 | 34.84 |
| | ATOM | 1518 | OE1 | GLN | A | 500 | 32.612 | 8.194 | 15.141 | 1.00 | 36.47 |
| 55 | ATOM | 1519 | NE2 | GLN | A | 500 | 33.301 | 10.324 | 15.082 | 1.00 | 38.25 |
| | ATOM | 1520 | C | GLN | A | 500 | 27.459 | 9.017 | 15.711 | 1.00 | 27.98 |
| | ATOM | 1521 | O | GLN | A | 500 | 26.700 | 8.469 | 14.908 | 1.00 | 24.84 |
| | ATOM | 1522 | N | HIS | A | 501 | 27.357 | 8.864 | 17.029 | 1.00 | 26.20 |
| | ATOM | 1523 | CA | HIS | A | 501 | 26.327 | 8.021 | 17.631 | 1.00 | 27.63 |
| 60 | ATOM | 1524 | CB | HIS | A | 501 | 26.535 | 7.919 | 19.145 | 1.00 | 27.97 |
| | ATOM | 1525 | CG | HIS | A | 501 | 27.892 | 7.420 | 19.535 | 1.00 | 34.27 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1526 | CD2 | HIS | A | 501 | 28.726 | 6.540 | 18.931 | 1.00 | 36.10 |
| | ATOM | 1527 | ND1 | HIS | A | 501 | 28.541 | 7.844 | 20.676 | 1.00 | 31.81 |
| | ATOM | 1528 | CE1 | HIS | A | 501 | 29.716 | 7.244 | 20.758 | 1.00 | 34.89 |
| | ATOM | 1529 | NE2 | HIS | A | 501 | 29.854 | 6.448 | 19.712 | 1.00 | 37.46 |
| | ATOM | 1530 | C | HIS | A | 501 | 24.935 | 8.572 | 17.348 | 1.00 | 24.93 |
| 10 | ATOM | 1531 | O | HIS | A | 501 | 23.998 | 7.815 | 17.107 | 1.00 | 26.73 |
| | ATOM | 1532 | N | GLN | A | 502 | 24.796 | 9.892 | 17.379 | 1.00 | 22.79 |
| | ATOM | 1533 | CA | GLN | A | 502 | 23.504 | 10.498 | 17.119 | 1.00 | 26.14 |
| | ATOM | 1534 | CB | GLN | A | 502 | 23.554 | 12.006 | 17.371 | 1.00 | 22.36 |
| | ATOM | 1535 | CG | GLN | A | 502 | 23.460 | 12.378 | 18.848 | 1.00 | 26.19 |
| 15 | ATOM | 1536 | CD | GLN | A | 502 | 23.589 | 13.875 | 19.089 | 1.00 | 28.67 |
| | ATOM | 1537 | OE1 | GLN | A | 502 | 23.632 | 14.663 | 18.149 | 1.00 | 28.40 |
| | ATOM | 1538 | NE2 | GLN | A | 502 | 23.651 | 14.268 | 20.355 | 1.00 | 24.72 |
| | ATOM | 1539 | C | GLN | A | 502 | 23.056 | 10.221 | 15.685 | 1.00 | 26.19 |
| | ATOM | 1540 | O | GLN | A | 502 | 21.913 | 9.822 | 15.453 | 1.00 | 24.09 |
| 20 | ATOM | 1541 | N | ARG | A | 503 | 23.955 | 10.429 | 14.727 | 1.00 | 24.88 |
| | ATOM | 1542 | CA | ARG | A | 503 | 23.630 | 10.196 | 13.326 | 1.00 | 25.25 |
| | ATOM | 1543 | CB | ARG | A | 503 | 24.772 | 10.668 | 12.418 | 1.00 | 27.63 |
| | ATOM | 1544 | CG | ARG | A | 503 | 24.432 | 10.563 | 10.932 | 1.00 | 28.75 |
| | ATOM | 1545 | CD | ARG | A | 503 | 25.479 | 11.222 | 10.056 | 1.00 | 27.72 |
| 25 | ATOM | 1546 | NE | ARG | A | 503 | 25.072 | 11.214 | 8.654 | 1.00 | 29.35 |
| | ATOM | 1547 | CZ | ARG | A | 503 | 24.279 | 12.126 | 8.105 | 1.00 | 25.84 |
| | ATOM | 1548 | NH1 | ARG | A | 503 | 23.804 | 13.120 | 8.840 | 1.00 | 27.35 |
| | ATOM | 1549 | NH2 | ARG | A | 503 | 23.962 | 12.044 | 6.820 | 1.00 | 30.63 |
| | ATOM | 1550 | C | ARG | A | 503 | 23.347 | 8.716 | 13.065 | 1.00 | 24.53 |
| 30 | ATOM | 1551 | O | ARG | A | 503 | 22.425 | 8.375 | 12.321 | 1.00 | 25.90 |
| | ATOM | 1552 | N | LEU | A | 504 | 24.143 | 7.841 | 13.672 | 1.00 | 23.00 |
| | ATOM | 1553 | CA | LEU | A | 504 | 23.953 | 6.406 | 13.496 | 1.00 | 22.60 |
| | ATOM | 1554 | CB | LEU | A | 504 | 24.971 | 5.621 | 14.323 | 1.00 | 25.43 |
| | ATOM | 1555 | CG | LEU | A | 504 | 24.781 | 4.100 | 14.344 | 1.00 | 25.23 |
| 35 | ATOM | 1556 | CD1 | LEU | A | 504 | 25.166 | 3.505 | 12.991 | 1.00 | 28.52 |
| | ATOM | 1557 | CD2 | LEU | A | 504 | 25.627 | 3.495 | 15.444 | 1.00 | 22.14 |
| | ATOM | 1558 | C | LEU | A | 504 | 22.541 | 6.030 | 13.934 | 1.00 | 22.84 |
| | ATOM | 1559 | O | LEU | A | 504 | 21.846 | 5.288 | 13.245 | 1.00 | 21.51 |
| | ATOM | 1560 | N | ALA | A | 505 | 22.120 | 6.547 | 15.083 | 1.00 | 20.16 |
| 40 | ATOM | 1561 | CA | ALA | A | 505 | 20.784 | 6.262 | 15.585 | 1.00 | 21.08 |
| | ATOM | 1562 | CB | ALA | A | 505 | 20.605 | 6.868 | 16.980 | 1.00 | 23.57 |
| | ATOM | 1563 | C | ALA | A | 505 | 19.738 | 6.832 | 14.628 | 1.00 | 20.20 |
| | ATOM | 1564 | O | ALA | A | 505 | 18.754 | 6.164 | 14.293 | 1.00 | 17.31 |
| | ATOM | 1565 | N | GLN | A | 506 | 19.954 | 8.066 | 14.184 | 1.00 | 22.11 |
| 45 | ATOM | 1566 | CA | GLN | A | 506 | 19.013 | 8.711 | 13.277 | 1.00 | 21.70 |
| | ATOM | 1567 | CB | GLN | A | 506 | 19.502 | 10.111 | 12.903 | 1.00 | 22.26 |
| | ATOM | 1568 | CG | GLN | A | 506 | 19.240 | 11.158 | 13.975 | 1.00 | 25.84 |
| | ATOM | 1569 | CD | GLN | A | 506 | 20.187 | 12.333 | 13.857 | 1.00 | 32.88 |
| | ATOM | 1570 | OE1 | GLN | A | 506 | 20.704 | 12.614 | 12.777 | 1.00 | 31.23 |
| 50 | ATOM | 1571 | NE2 | GLN | A | 506 | 20.423 | 13.025 | 14.968 | 1.00 | 32.97 |
| | ATOM | 1572 | C | GLN | A | 506 | 18.813 | 7.881 | 12.016 | 1.00 | 23.57 |
| | ATOM | 1573 | O | GLN | A | 506 | 17.684 | 7.715 | 11.550 | 1.00 | 21.83 |
| | ATOM | 1574 | N | LEU | A | 507 | 19.905 | 7.354 | 11.474 | 1.00 | 19.98 |
| | ATOM | 1575 | CA | LEU | A | 507 | 19.827 | 6.537 | 10.263 | 1.00 | 22.03 |
| 55 | ATOM | 1576 | CB | LEU | A | 507 | 21.231 | 6.244 | 9.725 | 1.00 | 23.02 |
| | ATOM | 1577 | CG | LEU | A | 507 | 22.026 | 7.457 | 9.225 | 1.00 | 25.80 |
| | ATOM | 1578 | CD1 | LEU | A | 507 | 23.371 | 6.994 | 8.713 | 1.00 | 27.67 |
| | ATOM | 1579 | CD2 | LEU | A | 507 | 21.264 | 8.176 | 8.130 | 1.00 | 25.62 |
| | ATOM | 1580 | C | LEU | A | 507 | 19.090 | 5.219 | 10.496 | 1.00 | 22.35 |
| 60 | ATOM | 1581 | O | LEU | A | 507 | 18.242 | 4.825 | 9.695 | 1.00 | 19.33 |
| | ATOM | 1582 | N | LEU | A | 508 | 19.402 | 4.539 | 11.592 | 1.00 | 21.29 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1583 | CA | LEU | A | 508 | 18.755 | 3.260 | 11.881 | 1.00 | 20.72 |
| | ATOM | 1584 | CB | LEU | A | 508 | 19.501 | 2.535 | 13.001 | 1.00 | 22.29 |
| | ATOM | 1585 | CG | LEU | A | 508 | 20.977 | 2.311 | 12.678 | 1.00 | 24.70 |
| | ATOM | 1586 | CD1 | LEU | A | 508 | 21.642 | 1.551 | 13.814 | 1.00 | 21.37 |
| | ATOM | 1587 | CD2 | LEU | A | 508 | 21.095 | 1.542 | 11.367 | 1.00 | 27.88 |
| 10 | ATOM | 1588 | C | LEU | A | 508 | 17.279 | 3.396 | 12.239 | 1.00 | 19.14 |
| | ATOM | 1589 | O | LEU | A | 508 | 16.498 | 2.478 | 12.003 | 1.00 | 17.80 |
| | ATOM | 1590 | N | LEU | A | 509 | 16.895 | 4.530 | 12.815 | 1.00 | 19.23 |
| | ATOM | 1591 | CA | LEU | A | 509 | 15.495 | 4.747 | 13.173 | 1.00 | 20.14 |
| | ATOM | 1592 | CB | LEU | A | 509 | 15.347 | 6.030 | 13.999 | 1.00 | 20.28 |
| 15 | ATOM | 1593 | CG | LEU | A | 509 | 15.710 | 5.858 | 15.479 | 1.00 | 21.35 |
| | ATOM | 1594 | CD1 | LEU | A | 509 | 15.354 | 7.106 | 16.263 | 1.00 | 19.29 |
| | ATOM | 1595 | CD2 | LEU | A | 509 | 14.989 | 4.656 | 16.038 | 1.00 | 20.84 |
| | ATOM | 1596 | C | LEU | A | 509 | 14.681 | 4.841 | 11.885 | 1.00 | 21.69 |
| | ATOM | 1597 | O | LEU | A | 509 | 13.493 | 4.514 | 11.854 | 1.00 | 22.40 |
| 20 | ATOM | 1598 | N | ILE | A | 510 | 15.343 | 5.270 | 10.815 | 1.00 | 20.22 |
| | ATOM | 1599 | CA | ILE | A | 510 | 14.710 | 5.397 | 9.508 | 1.00 | 20.40 |
| | ATOM | 1600 | CB | ILE | A | 510 | 15.720 | 5.946 | 8.464 | 1.00 | 28.34 |
| | ATOM | 1601 | CG2 | ILE | A | 510 | 15.208 | 5.710 | 7.056 | 1.00 | 32.54 |
| | ATOM | 1602 | CG1 | ILE | A | 510 | 15.965 | 7.438 | 8.696 | 1.00 | 28.23 |
| 25 | ATOM | 1603 | CD1 | ILE | A | 510 | 14.789 | 8.189 | 9.288 | 1.00 | 33.16 |
| | ATOM | 1604 | C | ILE | A | 510 | 14.210 | 4.025 | 9.049 | 1.00 | 23.21 |
| | ATOM | 1605 | O | ILE | A | 510 | 13.120 | 3.906 | 8.474 | 1.00 | 21.16 |
| | ATOM | 1606 | N | LEU | A | 511 | 14.998 | 2.989 | 9.323 | 1.00 | 18.38 |
| | ATOM | 1607 | CA | LEU | A | 511 | 14.633 | 1.634 | 8.917 | 1.00 | 20.10 |
| 30 | ATOM | 1608 | CB | LEU | A | 511 | 15.754 | 0.656 | 9.267 | 1.00 | 21.69 |
| | ATOM | 1609 | CG | LEU | A | 511 | 17.128 | 1.022 | 8.692 | 1.00 | 26.03 |
| | ATOM | 1610 | CD1 | LEU | A | 511 | 18.024 | -0.206 | 8.724 | 1.00 | 22.68 |
| | ATOM | 1611 | CD2 | LEU | A | 511 | 16.996 | 1.544 | 7.267 | 1.00 | 26.00 |
| | ATOM | 1612 | C | LEU | A | 511 | 13.326 | 1.181 | 9.543 | 1.00 | 18.51 |
| 35 | ATOM | 1613 | O | LEU | A | 511 | 12.663 | 0.283 | 9.025 | 1.00 | 17.40 |
| | ATOM | 1614 | N | SER | A | 512 | 12.963 | 1.799 | 10.664 | 1.00 | 18.68 |
| | ATOM | 1615 | CA | SER | A | 512 | 11.718 | 1.471 | 11.331 | 1.00 | 18.67 |
| | ATOM | 1616 | CB | SER | A | 512 | 11.661 | 2.117 | 12.720 | 1.00 | 18.58 |
| | ATOM | 1617 | OG | SER | A | 512 | 10.315 | 2.229 | 13.165 | 1.00 | 27.92 |
| 40 | ATOM | 1618 | C | SER | A | 512 | 10.572 | 1.994 | 10.464 | 1.00 | 18.43 |
| | ATOM | 1619 | O | SER | A | 512 | 9.584 | 1.296 | 10.236 | 1.00 | 13.91 |
| | ATOM | 1620 | N | HIS | A | 513 | 10.713 | 3.228 | 9.982 | 1.00 | 18.95 |
| | ATOM | 1621 | CA | HIS | A | 513 | 9.698 | 3.831 | 9.124 | 1.00 | 20.82 |
| | ATOM | 1622 | CB | HIS | A | 513 | 10.013 | 5.315 | 8.894 | 1.00 | 24.36 |
| 45 | ATOM | 1623 | CG | HIS | A | 513 | 9.923 | 6.146 | 10.136 | 1.00 | 32.13 |
| | ATOM | 1624 | CD2 | HIS | A | 513 | 8.863 | 6.744 | 10.734 | 1.00 | 35.29 |
| | ATOM | 1625 | ND1 | HIS | A | 513 | 11.010 | 6.391 | 10.949 | 1.00 | 35.00 |
| | ATOM | 1626 | CE1 | HIS | A | 513 | 10.624 | 7.101 | 11.995 | 1.00 | 34.67 |
| | ATOM | 1627 | NE2 | HIS | A | 513 | 9.326 | 7.328 | 11.889 | 1.00 | 35.82 |
| 50 | ATOM | 1628 | C | HIS | A | 513 | 9.650 | 3.079 | 7.790 | 1.00 | 19.08 |
| | ATOM | 1629 | O | HIS | A | 513 | 8.575 | 2.863 | 7.220 | 1.00 | 21.20 |
| | ATOM | 1630 | N | ILE | A | 514 | 10.809 | 2.662 | 7.297 | 1.00 | 15.58 |
| | ATOM | 1631 | CA | ILE | A | 514 | 10.849 | 1.921 | 6.038 | 1.00 | 16.48 |
| | ATOM | 1632 | CB | ILE | A | 514 | 12.312 | 1.678 | 5.576 | 1.00 | 20.09 |
| 55 | ATOM | 1633 | CG2 | ILE | A | 514 | 12.349 | 0.602 | 4.499 | 1.00 | 19.55 |
| | ATOM | 1634 | CG1 | ILE | A | 514 | 12.891 | 2.986 | 5.019 | 1.00 | 22.62 |
| | ATOM | 1635 | CD1 | ILE | A | 514 | 14.393 | 2.992 | 4.874 | 1.00 | 27.34 |
| | ATOM | 1636 | C | ILE | A | 514 | 10.112 | 0.590 | 6.210 | 1.00 | 16.40 |
| | ATOM | 1637 | O | ILE | A | 514 | 9.364 | 0.164 | 5.328 | 1.00 | 17.91 |
| 60 | ATOM | 1638 | N | ARG | A | 515 | 10.301 | -0.071 | 7.347 | 1.00 | 18.20 |
| | ATOM | 1639 | CA | ARG | A | 515 | 9.585 | -1.327 | 7.564 | 1.00 | 18.05 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1640 | CB | ARG | A | 515 | 9.984 | -1.980 | 8.889 | 1.00 | 18.36 |
| | ATOM | 1641 | CG | ARG | A | 515 | 9.173 | -3.237 | 9.213 | 1.00 | 17.84 |
| | ATOM | 1642 | CD | ARG | A | 515 | 9.823 | -4.470 | 8.606 | 1.00 | 17.94 |
| | ATOM | 1643 | NE | ARG | A | 515 | 11.038 | -4.813 | 9.334 | 1.00 | 26.96 |
| | ATOM | 1644 | CZ | ARG | A | 515 | 11.406 | -6.051 | 9.641 | 1.00 | 25.13 |
| 10 | ATOM | 1645 | NH1 | ARG | A | 515 | 10.654 | -7.080 | 9.281 | 1.00 | 23.49 |
| | ATOM | 1646 | NH2 | ARG | A | 515 | 12.511 | -6.254 | 10.340 | 1.00 | 32.16 |
| | ATOM | 1647 | C | ARG | A | 515 | 8.089 | -1.020 | 7.594 | 1.00 | 18.29 |
| | ATOM | 1648 | O | ARG | A | 515 | 7.275 | -1.759 | 7.038 | 1.00 | 16.22 |
| | ATOM | 1649 | N | HIS | A | 516 | 7.726 | 0.085 | 8.237 | 1.00 | 19.33 |
| 15 | ATOM | 1650 | CA | HIS | A | 516 | 6.317 | 0.441 | 8.330 | 1.00 | 17.78 |
| | ATOM | 1651 | CB | HIS | A | 516 | 6.126 | 1.702 | 9.166 | 1.00 | 16.84 |
| | ATOM | 1652 | CG | HIS | A | 516 | 4.692 | 2.101 | 9.312 | 1.00 | 18.16 |
| | ATOM | 1653 | CD2 | HIS | A | 516 | 3.967 | 3.061 | 8.691 | 1.00 | 21.17 |
| | ATOM | 1654 | ND1 | HIS | A | 516 | 3.830 | 1.469 | 10.180 | 1.00 | 20.70 |
| 20 | ATOM | 1655 | CE1 | HIS | A | 516 | 2.633 | 2.022 | 10.089 | 1.00 | 21.52 |
| | ATOM | 1656 | NE2 | HIS | A | 516 | 2.689 | 2.992 | 9.191 | 1.00 | 20.16 |
| | ATOM | 1657 | C | HIS | A | 516 | 5.708 | 0.659 | 6.954 | 1.00 | 16.63 |
| | ATOM | 1658 | O | HIS | A | 516 | 4.598 | 0.216 | 6.689 | 1.00 | 18.58 |
| | ATOM | 1659 | N | MET | A | 517 | 6.438 | 1.334 | 6.073 | 1.00 | 15.29 |
| 25 | ATOM | 1660 | CA | MET | A | 517 | 5.925 | 1.589 | 4.730 | 1.00 | 16.58 |
| | ATOM | 1661 | CB | MET | A | 517 | 6.837 | 2.576 | 4.002 | 1.00 | 18.66 |
| | ATOM | 1662 | CG | MET | A | 517 | 6.805 | 3.978 | 4.631 | 1.00 | 16.88 |
| | ATOM | 1663 | SD | MET | A | 517 | 7.670 | 5.243 | 3.701 | 1.00 | 24.08 |
| | ATOM | 1664 | CE | MET | A | 517 | 9.390 | 4.777 | 3.962 | 1.00 | 14.30 |
| 30 | ATOM | 1665 | C | MET | A | 517 | 5.773 | 0.289 | 3.940 | 1.00 | 17.86 |
| | ATOM | 1666 | O | MET | A | 517 | 4.791 | 0.101 | 3.224 | 1.00 | 18.25 |
| | ATOM | 1667 | N | SER | A | 518 | 6.741 | -0.610 | 4.086 | 1.00 | 17.43 |
| | ATOM | 1668 | CA | SER | A | 518 | 6.697 | -1.896 | 3.403 | 1.00 | 18.40 |
| | ATOM | 1669 | CB | SER | A | 518 | 7.974 | -2.695 | 3.680 | 1.00 | 16.77 |
| 35 | ATOM | 1670 | OG | SER | A | 518 | 7.834 | -4.030 | 3.227 | 1.00 | 24.23 |
| | ATOM | 1671 | C | SER | A | 518 | 5.476 | -2.695 | 3.854 | 1.00 | 17.91 |
| | ATOM | 1672 | O | SER | A | 518 | 4.788 | -3.295 | 3.030 | 1.00 | 18.97 |
| | ATOM | 1673 | N | ASN | A | 519 | 5.204 | -2.697 | 5.159 | 1.00 | 21.82 |
| | ATOM | 1674 | CA | ASN | A | 519 | 4.047 | -3.418 | 5.696 | 1.00 | 21.99 |
| 40 | ATOM | 1675 | CB | ASN | A | 519 | 3.957 | -3.257 | 7.216 | 1.00 | 23.24 |
| | ATOM | 1676 | CG | ASN | A | 519 | 5.046 | -4.011 | 7.957 | 1.00 | 31.14 |
| | ATOM | 1677 | OD1 | ASN | A | 519 | 5.585 | -4.999 | 7.461 | 1.00 | 32.50 |
| | ATOM | 1678 | ND2 | ASN | A | 519 | 5.368 | -3.545 | 9.163 | 1.00 | 29.10 |
| | ATOM | 1679 | C | ASN | A | 519 | 2.761 | -2.871 | 5.079 | 1.00 | 23.76 |
| 45 | ATOM | 1680 | O | ASN | A | 519 | 1.902 | -3.632 | 4.631 | 1.00 | 24.48 |
| | ATOM | 1681 | N | LYS | A | 520 | 2.627 | -1.548 | 5.078 | 1.00 | 20.58 |
| | ATOM | 1682 | CA | LYS | A | 520 | 1.449 | -0.900 | 4.512 | 1.00 | 25.49 |
| | ATOM | 1683 | CB | LYS | A | 520 | 1.484 | 0.607 | 4.786 | 1.00 | 24.73 |
| | ATOM | 1684 | CG | LYS | A | 520 | 1.512 | 0.996 | 6.264 | 1.00 | 32.31 |
| 50 | ATOM | 1685 | CD | LYS | A | 520 | 0.656 | 0.080 | 7.133 | 1.00 | 37.11 |
| | ATOM | 1686 | CE | LYS | A | 520 | -0.787 | 0.547 | 7.181 | 1.00 | 41.56 |
| | ATOM | 1687 | NZ | LYS | A | 520 | -1.560 | -0.134 | 8.261 | 1.00 | 42.66 |
| | ATOM | 1688 | C | LYS | A | 520 | 1.380 | -1.144 | 3.005 | 1.00 | 25.40 |
| | ATOM | 1689 | O | LYS | A | 520 | 0.316 | -1.436 | 2.467 | 1.00 | 26.44 |
| 55 | ATOM | 1690 | N | GLY | A | 521 | 2.520 | -1.021 | 2.332 | 1.00 | 22.88 |
| | ATOM | 1691 | CA | GLY | A | 521 | 2.561 | -1.236 | 0.897 | 1.00 | 21.53 |
| | ATOM | 1692 | C | GLY | A | 521 | 2.177 | -2.655 | 0.536 | 1.00 | 24.79 |
| | ATOM | 1693 | O | GLY | A | 521 | 1.426 | -2.878 | -0.413 | 1.00 | 25.71 |
| | ATOM | 1694 | N | MET | A | 522 | 2.696 | -3.619 | 1.290 | 1.00 | 22.75 |
| 60 | ATOM | 1695 | CA | MET | A | 522 | 2.393 | -5.027 | 1.058 | 1.00 | 23.40 |
| | ATOM | 1696 | CB | MET | A | 522 | 3.170 | -5.898 | 2.042 | 1.00 | 25.74 |

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 1697 | CG | MET | A | 522 | 3.396 | -7.308 | 1.559 | 1.00 | 31.06 |
| | ATOM | 1698 | SD | MET | A | 522 | 4.572 | -7.352 | 0.202 | 1.00 | 34.06 |
| | ATOM | 1699 | CE | MET | A | 522 | 6.125 | -7.229 | 1.113 | 1.00 | 29.28 |
| | ATOM | 1700 | C | MET | A | 522 | 0.893 | -5.281 | 1.218 | 1.00 | 26.49 |
| | ATOM | 1701 | O | MET | A | 522 | 0.268 | -5.920 | 0.361 | 1.00 | 25.47 |
| 10 | ATOM | 1702 | N | GLU | A | 523 | 0.321 | -4.790 | 2.318 | 1.00 | 24.95 |
| | ATOM | 1703 | CA | GLU | A | 523 | -1.110 | -4.954 | 2.566 | 1.00 | 27.15 |
| | ATOM | 1704 | CB | GLU | A | 523 | -1.555 | -4.206 | 3.835 | 1.00 | 31.08 |
| | ATOM | 1705 | CG | GLU | A | 523 | -0.830 | -4.564 | 5.124 | 1.00 | 38.93 |
| | ATOM | 1706 | CD | GLU | A | 523 | -1.153 | -3.585 | 6.258 | 1.00 | 46.90 |
| 15 | ATOM | 1707 | OE1 | GLU | A | 523 | -2.225 | -2.938 | 6.200 | 1.00 | 47.40 |
| | ATOM | 1708 | OE2 | GLU | A | 523 | -0.337 | -3.460 | 7.202 | 1.00 | 47.39 |
| | ATOM | 1709 | C | GLU | A | 523 | -1.872 | -4.368 | 1.381 | 1.00 | 26.10 |
| | ATOM | 1710 | O | GLU | A | 523 | -2.817 | -4.964 | 0.882 | 1.00 | 24.25 |
| | ATOM | 1711 | N | HIS | A | 524 | -1.449 | -3.182 | 0.940 | 1.00 | 24.74 |
| 20 | ATOM | 1712 | CA | HIS | A | 524 | -2.093 | -2.505 | -0.173 | 1.00 | 26.17 |
| | ATOM | 1713 | CB | HIS | A | 524 | -1.481 | -1.125 | -0.379 | 1.00 | 24.64 |
| | ATOM | 1714 | CG | HIS | A | 524 | -2.233 | -0.278 | -1.355 | 1.00 | 30.59 |
| | ATOM | 1715 | CD2 | HIS | A | 524 | -3.227 | 0.624 | -1.172 | 1.00 | 32.15 |
| | ATOM | 1716 | ND1 | HIS | A | 524 | -2.008 | -0.332 | -2.713 | 1.00 | 27.46 |
| 25 | ATOM | 1717 | CE1 | HIS | A | 524 | -2.829 | 0.502 | -3.326 | 1.00 | 34.58 |
| | ATOM | 1718 | NE2 | HIS | A | 524 | -3.580 | 1.094 | -2.413 | 1.00 | 30.50 |
| | ATOM | 1719 | C | HIS | A | 524 | -1.996 | -3.294 | -1.474 | 1.00 | 28.06 |
| | ATOM | 1720 | O | HIS | A | 524 | -2.976 | -3.419 | -2.217 | 1.00 | 29.81 |
| | ATOM | 1721 | N | LEU | A | 525 | -0.811 | -3.824 | -1.746 | 1.00 | 27.07 |
| 30 | ATOM | 1722 | CA | LEU | A | 525 | -0.594 | -4.601 | -2.955 | 1.00 | 29.30 |
| | ATOM | 1723 | CB | LEU | A | 525 | 0.865 | -5.039 | -3.051 | 1.00 | 26.39 |
| | ATOM | 1724 | CG | LEU | A | 525 | 1.307 | -5.765 | -4.321 | 1.00 | 29.34 |
| | ATOM | 1725 | CD1 | LEU | A | 525 | 0.734 | -5.076 | -5.562 | 1.00 | 29.61 |
| | ATOM | 1726 | CD2 | LEU | A | 525 | 2.829 | -5.769 | -4.370 | 1.00 | 29.22 |
| 35 | ATOM | 1727 | C | LEU | A | 525 | -1.497 | -5.822 | -2.950 | 1.00 | 31.67 |
| | ATOM | 1728 | O | LEU | A | 525 | -2.128 | -6.133 | -3.957 | 1.00 | 32.45 |
| | ATOM | 1729 | N | TYR | A | 526 | -1.559 | -6.512 | -1.814 | 1.00 | 36.14 |
| | ATOM | 1730 | CA | TYR | A | 526 | -2.397 | -7.698 | -1.696 | 1.00 | 40.36 |
| 40 | ATOM | 1731 | CB | TYR | A | 526 | -2.221 | -8.350 | -0.324 | 1.00 | 45.27 |
| | ATOM | 1732 | CG | TYR | A | 526 | -2.849 | -9.722 | -0.229 | 1.00 | 50.62 |
| | ATOM | 1733 | CD1 | TYR | A | 526 | -2.114 | -10.867 | -0.537 | 1.00 | 54.55 |
| | ATOM | 1734 | CE1 | TYR | A | 526 | -2.698 | -12.136 | -0.482 | 1.00 | 57.27 |
| | ATOM | 1735 | CD2 | TYR | A | 526 | -4.188 | -9.876 | 0.142 | 1.00 | 53.48 |
| | ATOM | 1736 | CE2 | TYR | A | 526 | -4.781 | -11.141 | 0.201 | 1.00 | 55.93 |
| 45 | ATOM | 1737 | CZ | TYR | A | 526 | -4.029 | -12.264 | -0.113 | 1.00 | 56.60 |
| | ATOM | 1738 | OH | TYR | A | 526 | -4.603 | -13.515 | -0.063 | 1.00 | 60.70 |
| | ATOM | 1739 | C | TYR | A | 526 | -3.852 | -7.298 | -1.893 | 1.00 | 42.83 |
| | ATOM | 1740 | O | TYR | A | 526 | -4.673 | -8.094 | -2.349 | 1.00 | 43.49 |
| 50 | ATOM | 1741 | N | SER | A | 527 | -4.158 | -6.055 | -1.543 | 1.00 | 41.55 |
| | ATOM | 1742 | CA | SER | A | 527 | -5.503 | -5.523 | -1.686 | 1.00 | 44.04 |
| | ATOM | 1743 | CB | SER | A | 527 | -5.606 | -4.169 | -0.979 | 1.00 | 43.47 |
| | ATOM | 1744 | OG | SER | A | 527 | -6.954 | -3.789 | -0.786 | 1.00 | 47.51 |
| | ATOM | 1745 | C | SER | A | 527 | -5.817 | -5.356 | -3.172 | 1.00 | 44.18 |
| | ATOM | 1746 | O | SER | A | 527 | -6.883 | -5.757 | -3.642 | 1.00 | 44.88 |
| 55 | ATOM | 1747 | N | MET | A | 528 | -4.883 | -4.755 | -3.901 | 1.00 | 41.79 |
| | ATOM | 1748 | CA | MET | A | 528 | -5.047 | -4.536 | -5.331 | 1.00 | 44.04 |
| | ATOM | 1749 | CB | MET | A | 528 | -3.898 | -3.679 | -5.870 | 1.00 | 44.78 |
| | ATOM | 1750 | CG | MET | A | 528 | -3.965 | -2.206 | -5.468 | 1.00 | 45.37 |
| | ATOM | 1751 | SD | MET | A | 528 | -5.652 | -1.598 | -5.273 | 1.00 | 51.83 |
| 60 | ATOM | 1752 | CE | MET | A | 528 | -5.553 | -0.004 | -6.044 | 1.00 | 46.61 |
| | ATOM | 1753 | C | MET | A | 528 | -5.087 | -5.871 | -6.071 | 1.00 | 44.29 |

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|----|------|------|-----|-----|---|-----|--------|---------|---------|------|-------|
| 5 | ATOM | 1754 | O | MET | A | 528 | -5.689 | -5.979 | -7.137 | 1.00 | 44.02 |
| | ATOM | 1755 | N | LYS | A | 529 | -4.443 | -6.883 | -5.499 | 1.00 | 46.78 |
| | ATOM | 1756 | CA | LYS | A | 529 | -4.413 | -8.213 | -6.099 | 1.00 | 51.28 |
| | ATOM | 1757 | CB | LYS | A | 529 | -3.550 | -9.158 | -5.261 | 1.00 | 50.87 |
| | ATOM | 1758 | CG | LYS | A | 529 | -2.798 | -10.204 | -6.071 | 1.00 | 50.55 |
| 10 | ATOM | 1759 | CD | LYS | A | 529 | -3.548 | -11.520 | -6.104 | 1.00 | 51.25 |
| | ATOM | 1760 | CE | LYS | A | 529 | -2.616 | -12.694 | -5.856 | 1.00 | 53.22 |
| | ATOM | 1761 | NZ | LYS | A | 529 | -2.420 | -12.954 | -4.402 | 1.00 | 53.22 |
| | ATOM | 1762 | C | LYS | A | 529 | -5.829 | -8.768 | -6.182 | 1.00 | 54.27 |
| | ATOM | 1763 | O | LYS | A | 529 | -6.325 | -9.069 | -7.266 | 1.00 | 55.50 |
| 15 | ATOM | 1764 | N | CYS | A | 530 | -6.472 | -8.901 | -5.027 | 1.00 | 56.71 |
| | ATOM | 1765 | CA | CYS | A | 530 | -7.833 | -9.416 | -4.961 | 1.00 | 58.35 |
| | ATOM | 1766 | CB | CYS | A | 530 | -8.333 | -9.380 | -3.517 | 1.00 | 59.78 |
| | ATOM | 1767 | SG | CYS | A | 530 | -7.289 | -10.304 | -2.358 | 1.00 | 63.19 |
| | ATOM | 1768 | C | CYS | A | 530 | -8.766 | -8.609 | -5.858 | 1.00 | 59.36 |
| 20 | ATOM | 1769 | O | CYS | A | 530 | -9.644 | -9.169 | -6.514 | 1.00 | 59.52 |
| | ATOM | 1770 | N | LYS | A | 531 | -8.569 | -7.293 | -5.888 | 1.00 | 59.24 |
| | ATOM | 1771 | CA | LYS | A | 531 | -9.390 | -6.411 | -6.713 | 1.00 | 60.14 |
| | ATOM | 1772 | CB | LYS | A | 531 | -9.158 | -4.952 | -6.317 | 1.00 | 58.92 |
| | ATOM | 1773 | C | LYS | A | 531 | -9.073 | -6.615 | -8.195 | 1.00 | 61.48 |
| 25 | ATOM | 1774 | O | LYS | A | 531 | -9.618 | -5.928 | -9.061 | 1.00 | 61.74 |
| | ATOM | 1775 | N | ASN | A | 532 | -8.179 | -7.561 | -8.474 | 1.00 | 61.65 |
| | ATOM | 1776 | CA | ASN | A | 532 | -7.783 | -7.890 | -9.840 | 1.00 | 61.60 |
| | ATOM | 1777 | CB | ASN | A | 532 | -8.966 | -8.518 | -10.581 | 1.00 | 62.28 |
| | ATOM | 1778 | CG | ASN | A | 532 | -8.750 | -9.985 | -10.878 | 1.00 | 64.66 |
| 30 | ATOM | 1779 | OD1 | ASN | A | 532 | -8.344 | -10.352 | -11.983 | 1.00 | 67.08 |
| | ATOM | 1780 | ND2 | ASN | A | 532 | -9.016 | -10.836 | -9.891 | 1.00 | 62.68 |
| | ATOM | 1781 | C | ASN | A | 532 | -7.247 | -6.710 | -10.648 | 1.00 | 59.75 |
| | ATOM | 1782 | O | ASN | A | 532 | -7.487 | -6.615 | -11.850 | 1.00 | 57.50 |
| | ATOM | 1783 | N | VAL | A | 533 | -6.507 | -5.822 | -9.992 | 1.00 | 59.39 |
| 35 | ATOM | 1784 | CA | VAL | A | 533 | -5.954 | -4.656 | -10.669 | 1.00 | 58.22 |
| | ATOM | 1785 | CB | VAL | A | 533 | -6.223 | -3.371 | -9.865 | 1.00 | 59.20 |
| | ATOM | 1786 | CG1 | VAL | A | 533 | -6.181 | -2.163 | -10.785 | 1.00 | 59.21 |
| | ATOM | 1787 | CG2 | VAL | A | 533 | -7.574 | -3.467 | -9.172 | 1.00 | 59.57 |
| | ATOM | 1788 | C | VAL | A | 533 | -4.452 | -4.767 | -10.907 | 1.00 | 57.86 |
| 40 | ATOM | 1789 | O | VAL | A | 533 | -3.846 | -3.874 | -11.499 | 1.00 | 60.56 |
| | ATOM | 1790 | N | VAL | A | 534 | -3.852 | -5.863 | -10.451 | 1.00 | 56.03 |
| | ATOM | 1791 | CA | VAL | A | 534 | -2.417 | -6.063 | -10.621 | 1.00 | 54.11 |
| | ATOM | 1792 | CB | VAL | A | 534 | -1.767 | -6.632 | -9.341 | 1.00 | 54.02 |
| | ATOM | 1793 | CG1 | VAL | A | 534 | -0.300 | -6.950 | -9.601 | 1.00 | 52.37 |
| 45 | ATOM | 1794 | CG2 | VAL | A | 534 | -1.900 | -5.635 | -8.200 | 1.00 | 55.70 |
| | ATOM | 1795 | C | VAL | A | 534 | -2.089 | -7.008 | -11.770 | 1.00 | 54.31 |
| | ATOM | 1796 | O | VAL | A | 534 | -2.519 | -8.164 | -11.780 | 1.00 | 51.66 |
| | ATOM | 1797 | N | PRO | A | 535 | -1.315 | -6.527 | -12.755 | 1.00 | 53.54 |
| | ATOM | 1798 | CD | PRO | A | 535 | -0.749 | -5.172 | -12.874 | 1.00 | 54.28 |
| 50 | ATOM | 1799 | CA | PRO | A | 535 | -0.949 | -7.373 | -13.893 | 1.00 | 53.24 |
| | ATOM | 1800 | CB | PRO | A | 535 | 0.011 | -6.500 | -14.697 | 1.00 | 52.71 |
| | ATOM | 1801 | CG | PRO | A | 535 | -0.353 | -5.102 | -14.319 | 1.00 | 53.19 |
| | ATOM | 1802 | C | PRO | A | 535 | -0.296 | -8.664 | -13.411 | 1.00 | 54.25 |
| | ATOM | 1803 | O | PRO | A | 535 | 0.121 | -8.768 | -12.254 | 1.00 | 54.56 |
| 55 | ATOM | 1804 | N | LEU | A | 536 | -0.203 | -9.645 | -14.299 | 1.00 | 53.63 |
| | ATOM | 1805 | CA | LEU | A | 536 | 0.382 | -10.926 | -13.937 | 1.00 | 53.11 |
| | ATOM | 1806 | CB | LEU | A | 536 | -0.250 | -12.046 | -14.763 | 1.00 | 51.88 |
| | ATOM | 1807 | CG | LEU | A | 536 | -0.686 | -13.256 | -13.938 | 1.00 | 51.83 |
| | ATOM | 1808 | CD1 | LEU | A | 536 | -1.953 | -12.917 | -13.173 | 1.00 | 49.51 |
| 60 | ATOM | 1809 | CD2 | LEU | A | 536 | -0.905 | -14.449 | -14.854 | 1.00 | 53.43 |
| | ATOM | 1810 | C | LEU | A | 536 | 1.895 | -10.990 | -14.081 | 1.00 | 52.58 |

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|----|------|------|-----|-----|---|-----|--------|----------------|------|-------|
| 5 | ATOM | 1811 | O | LEU | A | 536 | 2.414 | -11.501-15.075 | 1.00 | 55.33 |
| | ATOM | 1812 | N | TYR | A | 537 | 2.601 | -10.462-13.087 | 1.00 | 48.72 |
| | ATOM | 1813 | CA | TYR | A | 537 | 4.057 | -10.501-13.093 | 1.00 | 44.22 |
| | ATOM | 1814 | CB | TYR | A | 537 | 4.627 | -9.134-12.709 | 1.00 | 44.52 |
| | ATOM | 1815 | CG | TYR | A | 537 | 4.331 | -8.053-13.731 | 1.00 | 45.18 |
| 10 | ATOM | 1816 | CD1 | TYR | A | 537 | 3.623 | -6.905-13.376 | 1.00 | 43.77 |
| | ATOM | 1817 | CE1 | TYR | A | 537 | 3.334 | -5.915-14.317 | 1.00 | 45.23 |
| | ATOM | 1818 | CD2 | TYR | A | 537 | 4.747 | -8.187-15.058 | 1.00 | 46.91 |
| | ATOM | 1819 | CE2 | TYR | A | 537 | 4.462 | -7.202-16.008 | 1.00 | 43.93 |
| | ATOM | 1820 | CZ | TYR | A | 537 | 3.757 | -6.071-15.631 | 1.00 | 46.70 |
| 15 | ATOM | 1821 | OH | TYR | A | 537 | 3.472 | -5.097-16.565 | 1.00 | 48.35 |
| | ATOM | 1822 | C | TYR | A | 537 | 4.401 | -11.562-12.056 | 1.00 | 41.29 |
| | ATOM | 1823 | O | TYR | A | 537 | 4.330 | -11.319-10.856 | 1.00 | 41.82 |
| | ATOM | 1824 | N | ASP | A | 538 | 4.748 | -12.748-12.540 | 1.00 | 40.34 |
| 20 | ATOM | 1825 | CA | ASP | A | 538 | 5.055 | -13.896-11.691 | 1.00 | 38.84 |
| | ATOM | 1826 | CB | ASP | A | 538 | 5.594 | -15.037-12.554 | 1.00 | 43.47 |
| | ATOM | 1827 | CG | ASP | A | 538 | 4.571 | -15.531-13.566 | 1.00 | 47.67 |
| | ATOM | 1828 | OD1 | ASP | A | 538 | 4.931 | -16.373-14.416 | 1.00 | 49.33 |
| | ATOM | 1829 | OD2 | ASP | A | 538 | 3.405 | -15.073-13.511 | 1.00 | 48.07 |
| 25 | ATOM | 1830 | C | ASP | A | 538 | 5.991 | -13.676-10.508 | 1.00 | 37.28 |
| | ATOM | 1831 | O | ASP | A | 538 | 5.620 | -13.964-9.371 | 1.00 | 38.55 |
| | ATOM | 1832 | N | LEU | A | 539 | 7.196 | -13.200-10.766 | 1.00 | 33.83 |
| | ATOM | 1833 | CA | LEU | A | 539 | 8.155 | -12.959-9.692 | 1.00 | 32.80 |
| | ATOM | 1834 | CB | LEU | A | 539 | 9.419 | -12.323-10.263 | 1.00 | 32.78 |
| | ATOM | 1835 | CG | LEU | A | 539 | 10.561 | -12.031-9.292 | 1.00 | 30.93 |
| 30 | ATOM | 1836 | CD1 | LEU | A | 539 | 10.913 | -13.280-8.492 | 1.00 | 33.81 |
| | ATOM | 1837 | CD2 | LEU | A | 539 | 11.758 | -11.538-10.077 | 1.00 | 25.92 |
| | ATOM | 1838 | C | LEU | A | 539 | 7.558 | -12.050-8.614 | 1.00 | 31.85 |
| | ATOM | 1839 | O | LEU | A | 539 | 7.590 | -12.367-7.423 | 1.00 | 25.63 |
| | ATOM | 1840 | N | LEU | A | 540 | 7.011 | -10.917-9.042 | 1.00 | 32.07 |
| 35 | ATOM | 1841 | CA | LEU | A | 540 | 6.411 | -9.976-8.111 | 1.00 | 31.03 |
| | ATOM | 1842 | CB | LEU | A | 540 | 5.792 | -8.800-8.861 | 1.00 | 30.56 |
| | ATOM | 1843 | CG | LEU | A | 540 | 5.124 | -7.774-7.945 | 1.00 | 31.12 |
| | ATOM | 1844 | CD1 | LEU | A | 540 | 6.092 | -7.357-6.838 | 1.00 | 29.76 |
| | ATOM | 1845 | CD2 | LEU | A | 540 | 4.693 | -6.572-8.762 | 1.00 | 30.85 |
| 40 | ATOM | 1846 | C | LEU | A | 540 | 5.337 | -10.660-7.282 | 1.00 | 34.55 |
| | ATOM | 1847 | O | LEU | A | 540 | 5.316 | -10.522-6.063 | 1.00 | 31.60 |
| | ATOM | 1848 | N | LEU | A | 541 | 4.446 | -11.388-7.941 | 1.00 | 35.64 |
| | ATOM | 1849 | CA | LEU | A | 541 | 3.378 | -12.101-7.245 | 1.00 | 37.84 |
| | ATOM | 1850 | CB | LEU | A | 541 | 2.452 | -12.771-8.255 | 1.00 | 38.49 |
| 45 | ATOM | 1851 | CG | LEU | A | 541 | 1.244 | -11.932-8.678 | 1.00 | 39.80 |
| | ATOM | 1852 | CD1 | LEU | A | 541 | 0.476 | -11.476-7.448 | 1.00 | 40.02 |
| | ATOM | 1853 | CD2 | LEU | A | 541 | 1.713 | -10.733-9.485 | 1.00 | 40.48 |
| | ATOM | 1854 | C | LEU | A | 541 | 3.937 | -13.147-6.275 | 1.00 | 40.10 |
| | ATOM | 1855 | O | LEU | A | 541 | 3.472 | -13.254-5.137 | 1.00 | 42.72 |
| 50 | ATOM | 1856 | N | GLU | A | 542 | 4.929 | -13.915-6.723 | 1.00 | 38.45 |
| | ATOM | 1857 | CA | GLU | A | 542 | 5.535 | -14.932-5.868 | 1.00 | 39.59 |
| | ATOM | 1858 | CB | GLU | A | 542 | 6.738 | -15.566-6.564 | 1.00 | 41.73 |
| | ATOM | 1859 | CG | GLU | A | 542 | 6.396 | -16.327-7.831 | 1.00 | 48.34 |
| | ATOM | 1860 | CD | GLU | A | 542 | 6.931 | -17.747-7.819 | 1.00 | 52.57 |
| 55 | ATOM | 1861 | OE1 | GLU | A | 542 | 8.049 | -17.961-7.298 | 1.00 | 52.70 |
| | ATOM | 1862 | OE2 | GLU | A | 542 | 6.230 | -18.647-8.331 | 1.00 | 53.69 |
| | ATOM | 1863 | C | GLU | A | 542 | 5.989 | -14.299-4.553 | 1.00 | 39.94 |
| | ATOM | 1864 | O | GLU | A | 542 | 5.567 | -14.710-3.472 | 1.00 | 40.99 |
| | ATOM | 1865 | N | MET | A | 543 | 6.844 | -13.287-4.663 | 1.00 | 38.29 |
| 60 | ATOM | 1866 | CA | MET | A | 543 | 7.380 | -12.580-3.503 | 1.00 | 38.11 |
| | ATOM | 1867 | CB | MET | A | 543 | 8.242 | -11.408-3.963 | 1.00 | 37.34 |

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|----|--------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 1868 | CG | MET | A | 543 | 9.311 | -11.797 | -4.953 | 1.00 | 40.59 |
| | ATOM | 1869 | SD | MET | A | 543 | 10.829 | -12.223 | -4.114 | 1.00 | 45.64 |
| | ATOM | 1870 | CE | MET | A | 543 | 12.014 | -11.399 | -5.151 | 1.00 | 42.61 |
| | ATOM | 1871 | C | MET | A | 543 | 6.287 | -12.064 | -2.581 | 1.00 | 37.94 |
| 10 | ATOM | 1872 | O | MET | A | 543 | 6.413 | -12.127 | -1.358 | 1.00 | 39.20 |
| | ATOM | 1873 | N | LEU | A | 544 | 5.218 | -11.544 | -3.175 | 1.00 | 39.44 |
| | ATOM | 1874 | CA | LEU | A | 544 | 4.100 | -11.013 | -2.408 | 1.00 | 40.91 |
| | ATOM | 1875 | CB | LEU | A | 544 | 3.087 | -10.344 | -3.341 | 1.00 | 39.88 |
| 15 | ATOM | 1876 | CG | LEU | A | 544 | 1.775 | -9.905 | -2.688 | 1.00 | 42.70 |
| | ATOM | 1877 | CD1 | LEU | A | 544 | 2.060 | -8.886 | -1.586 | 1.00 | 37.35 |
| | ATOM | 1878 | CD2 | LEU | A | 544 | 0.854 | -9.317 | -3.741 | 1.00 | 38.47 |
| | ATOM | 1879 | C | LEU | A | 544 | 3.420 | -12.120 | -1.614 | 1.00 | 42.83 |
| 20 | ATOM | 1880 | O | LEU | A | 544 | 2.957 | -11.899 | -0.496 | 1.00 | 42.73 |
| | ATOM | 1881 | N | ASP | A | 545 | 3.367 | -13.313 | -2.197 | 1.00 | 46.32 |
| | ATOM | 1882 | CA | ASP | A | 545 | 2.746 | -14.456 | -1.539 | 1.00 | 50.65 |
| | ATOM | 1883 | CB | ASP | A | 545 | 2.606 | -15.617 | -2.524 | 1.00 | 53.67 |
| 25 | ATOM | 1884 | CG | ASP | A | 545 | 1.703 | -15.278 | -3.691 | 1.00 | 57.35 |
| | ATOM | 1885 | OD1 | ASP | A | 545 | 0.697 | -14.568 | -3.475 | 1.00 | 59.99 |
| | ATOM | 1886 | OD2 | ASP | A | 545 | 1.999 | -15.718 | -4.824 | 1.00 | 59.68 |
| | ATOM | 1887 | C | ASP | A | 545 | 3.559 | -14.898 | -0.327 | 1.00 | 50.74 |
| 30 | ATOM | 1888 | O | ASP | A | 545 | 3.004 | -15.388 | 0.657 | 1.00 | 49.39 |
| | ATOM | 1889 | N | ALA | A | 546 | 4.874 | -14.723 | -0.401 | 1.00 | 51.82 |
| | ATOM | 1890 | CA | ALA | A | 546 | 5.750 | -15.095 | 0.702 | 1.00 | 53.12 |
| | ATOM | 1891 | CB | ALA | A | 546 | 7.180 | -14.678 | 0.395 | 1.00 | 53.19 |
| 35 | ATOM | 1892 | C | ALA | A | 546 | 5.269 | -14.424 | 1.987 | 1.00 | 54.67 |
| | ATOM | 1893 | O | ALA | A | 546 | 5.476 | -14.940 | 3.085 | 1.00 | 52.32 |
| | ATOM | 1894 | N | HIS | A | 547 | 4.622 | -13.270 | 1.838 | 1.00 | 56.66 |
| | ATOM | 1895 | CA | HIS | A | 547 | 4.102 | -12.520 | 2.978 | 1.00 | 59.19 |
| 40 | ATOM | 1896 | CB | HIS | A | 547 | 4.144 | -11.017 | 2.684 | 1.00 | 56.70 |
| | ATOM | 1897 | CG | HIS | A | 547 | 5.489 | -10.394 | 2.896 | 1.00 | 54.64 |
| | ATOM | 1898 | CD2 | HIS | A | 547 | 6.644 | -10.506 | 2.199 | 1.00 | 53.92 |
| | ATOM | 1899 | ND1 | HIS | A | 547 | 5.748 | -9.514 | 3.925 | 1.00 | 52.17 |
| 45 | ATOM | 1900 | CE1 | HIS | A | 547 | 7.004 | -9.111 | 3.853 | 1.00 | 52.16 |
| | ATOM | 1901 | NE2 | HIS | A | 547 | 7.570 | -9.698 | 2.814 | 1.00 | 51.90 |
| | ATOM | 1902 | C | HIS | A | 547 | 2.668 | -12.940 | 3.306 | 1.00 | 62.77 |
| | ATOM | 1903 | O | HIS | A | 547 | 1.842 | -12.120 | 3.707 | 1.00 | 63.24 |
| 50 | ATOM | 1904 | N | ARG | A | 548 | 2.381 | -14.224 | 3.133 | 1.00 | 68.37 |
| | ATOM | 1905 | CA | ARG | A | 548 | 1.053 | -14.758 | 3.411 | 1.00 | 72.75 |
| | ATOM | 1906 | CB | ARG | A | 548 | 0.243 | -14.864 | 2.113 | 1.00 | 73.73 |
| | ATOM | 1907 | CG | ARG | A | 548 | -1.149 | -14.243 | 2.186 | 1.00 | 74.04 |
| 55 | ATOM | 1908 | CD | ARG | A | 548 | -1.081 | -12.728 | 2.297 | 1.00 | 74.50 |
| | ATOM | 1909 | NE | ARG | A | 548 | -2.305 | -12.167 | 2.863 | 1.00 | 75.04 |
| | ATOM | 1910 | CZ | ARG | A | 548 | -2.478 | -10.880 | 3.149 | 1.00 | 75.59 |
| | ATOM | 1911 | NH1 | ARG | A | 548 | -1.506 | -10.006 | 2.919 | 1.00 | 75.79 |
| 60 | ATOM | 1912 | NH2 | ARG | A | 548 | -3.627 | -10.464 | 3.662 | 1.00 | 76.00 |
| | ATOM | 1913 | C | ARG | A | 548 | 1.179 | -16.133 | 4.061 | 1.00 | 74.94 |
| | ATOM | 1914 | O | ARG | A | 548 | 0.197 | -16.697 | 4.549 | 1.00 | 75.15 |
| | ATOM | 1915 | N | LEU | A | 549 | 2.398 | -16.665 | 4.063 | 1.00 | 76.49 |
| 65 | ATOM | 1916 | CA | LEU | A | 549 | 2.669 | -17.969 | 4.653 | 1.00 | 78.14 |
| | ATOM | 1917 | CB | LEU | A | 549 | 2.971 | -18.986 | 3.557 | 1.00 | 77.55 |
| | ATOM | 1918 | C | LEU | A | 549 | 3.846 | -17.870 | 5.619 | 1.00 | 79.13 |
| | ATOM | 1919 | O | LEU | A | 549 | 4.892 | -17.317 | 5.215 | 1.00 | 80.40 |
| 70 | ATOM | 1920 | OXT | LEU | A | 549 | 3.708 | -18.341 | 6.769 | 1.00 | 79.46 |
| | HETATM | 1921 | CP9 | DES | A | 600 | 5.390 | -3.061 | -6.139 | 1.00 | 21.38 |
| | HETATM | 1922 | CP8 | DES | A | 600 | 5.834 | -1.989 | -5.134 | 1.00 | 22.41 |
| | HETATM | 1923 | CP7 | DES | A | 600 | 5.038 | -0.714 | -5.236 | 1.00 | 21.32 |
| 75 | HETATM | 1924 | CP6 | DES | A | 600 | 3.587 | -0.864 | -5.062 | 1.00 | 25.87 |

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|----|--------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| 5 | HETATM | 1925 | CP1 | DES | A | 600 | 2.987 | -0.978 | -3.784 | 1.00 | 23.92 |
| | HETATM | 1926 | CP2 | DES | A | 600 | 1.597 | -1.150 | -3.684 | 1.00 | 29.77 |
| | HETATM | 1927 | CP3 | DES | A | 600 | 0.842 | -1.214 | -4.871 | 1.00 | 31.40 |
| | HETATM | 1928 | OP3 | DES | A | 600 | -0.506 | -1.419 | -4.824 | 1.00 | 33.36 |
| | HETATM | 1929 | CP4 | DES | A | 600 | 1.421 | -1.099 | -6.143 | 1.00 | 27.01 |
| 10 | HETATM | 1930 | CP5 | DES | A | 600 | 2.793 | -0.929 | -6.230 | 1.00 | 27.40 |
| | HETATM | 1931 | C7 | DES | A | 600 | 5.671 | 0.461 | -5.482 | 1.00 | 22.39 |
| | HETATM | 1932 | C6 | DES | A | 600 | 7.113 | 0.561 | -5.809 | 1.00 | 21.75 |
| | HETATM | 1933 | C5 | DES | A | 600 | 7.541 | 0.306 | -7.131 | 1.00 | 19.97 |
| | HETATM | 1934 | C4 | DES | A | 600 | 8.889 | 0.429 | -7.477 | 1.00 | 23.81 |
| 15 | HETATM | 1935 | C3 | DES | A | 600 | 9.814 | 0.804 | -6.488 | 1.00 | 21.88 |
| | HETATM | 1936 | O3 | DES | A | 600 | 11.125 | 0.901 | -6.839 | 1.00 | 22.32 |
| | HETATM | 1937 | C2 | DES | A | 600 | 9.423 | 1.066 | -5.161 | 1.00 | 19.74 |
| | HETATM | 1938 | C1 | DES | A | 600 | 8.066 | 0.937 | -4.838 | 1.00 | 21.25 |
| | HETATM | 1939 | C8 | DES | A | 600 | 4.894 | 1.765 | -5.443 | 1.00 | 21.47 |
| 20 | HETATM | 1940 | C9 | DES | A | 600 | 4.959 | 2.468 | -4.070 | 1.00 | 21.38 |
| | HETATM | 1941 | CL | CL | A | 601 | 14.781 | -3.035 | -17.739 | 1.00 | 24.10 |
| | ATOM | 1942 | CB | SER | B | 305 | 12.321 | 21.086 | 25.295 | 1.00 | 64.27 |
| | ATOM | 1943 | C | SER | B | 305 | 12.672 | 22.102 | 27.548 | 1.00 | 64.37 |
| | ATOM | 1944 | O | SER | B | 305 | 13.701 | 22.760 | 27.702 | 1.00 | 66.90 |
| 25 | ATOM | 1945 | N | SER | B | 305 | 12.045 | 23.521 | 25.606 | 1.00 | 63.72 |
| | ATOM | 1946 | CA | SER | B | 305 | 11.875 | 22.187 | 26.251 | 1.00 | 64.21 |
| | ATOM | 1947 | N | LEU | B | 306 | 12.193 | 21.293 | 28.484 | 1.00 | 63.09 |
| | ATOM | 1948 | CA | LEU | B | 306 | 12.884 | 21.133 | 29.757 | 1.00 | 60.98 |
| | ATOM | 1949 | CB | LEU | B | 306 | 11.884 | 21.200 | 30.913 | 1.00 | 61.23 |
| 30 | ATOM | 1950 | CG | LEU | B | 306 | 12.221 | 20.417 | 32.183 | 1.00 | 62.23 |
| | ATOM | 1951 | CD1 | LEU | B | 306 | 13.304 | 21.144 | 32.966 | 1.00 | 62.56 |
| | ATOM | 1952 | CD2 | LEU | B | 306 | 10.965 | 20.258 | 33.027 | 1.00 | 64.31 |
| | ATOM | 1953 | C | LEU | B | 306 | 13.660 | 19.819 | 29.803 | 1.00 | 58.39 |
| | ATOM | 1954 | O | LEU | B | 306 | 14.570 | 19.654 | 30.614 | 1.00 | 58.56 |
| 35 | ATOM | 1955 | N | ALA | B | 307 | 13.293 | 18.881 | 28.933 | 1.00 | 54.82 |
| | ATOM | 1956 | CA | ALA | B | 307 | 13.971 | 17.589 | 28.861 | 1.00 | 50.62 |
| | ATOM | 1957 | CB | ALA | B | 307 | 13.092 | 16.584 | 28.143 | 1.00 | 51.30 |
| | ATOM | 1958 | C | ALA | B | 307 | 15.303 | 17.719 | 28.122 | 1.00 | 46.84 |
| | ATOM | 1959 | O | ALA | B | 307 | 16.196 | 16.885 | 28.274 | 1.00 | 45.62 |
| 40 | ATOM | 1960 | N | LEU | B | 308 | 15.431 | 18.769 | 27.320 | 1.00 | 43.46 |
| | ATOM | 1961 | CA | LEU | B | 308 | 16.643 | 18.983 | 26.542 | 1.00 | 43.01 |
| | ATOM | 1962 | CB | LEU | B | 308 | 16.413 | 20.100 | 25.526 | 1.00 | 41.32 |
| | ATOM | 1963 | CG | LEU | B | 308 | 16.315 | 19.708 | 24.051 | 1.00 | 43.10 |
| | ATOM | 1964 | CD1 | LEU | B | 308 | 15.942 | 18.239 | 23.903 | 1.00 | 40.51 |
| 45 | ATOM | 1965 | CD2 | LEU | B | 308 | 15.287 | 20.602 | 23.375 | 1.00 | 39.80 |
| | ATOM | 1966 | C | LEU | B | 308 | 17.874 | 19.297 | 27.385 | 1.00 | 42.11 |
| | ATOM | 1967 | O | LEU | B | 308 | 19.000 | 19.102 | 26.932 | 1.00 | 44.34 |
| | ATOM | 1968 | N | SER | B | 309 | 17.669 | 19.775 | 28.608 | 1.00 | 40.88 |
| | ATOM | 1969 | CA | SER | B | 309 | 18.796 | 20.100 | 29.475 | 1.00 | 42.79 |
| 50 | ATOM | 1970 | CB | SER | B | 309 | 18.562 | 21.447 | 30.163 | 1.00 | 41.25 |
| | ATOM | 1971 | OG | SER | B | 309 | 17.459 | 21.379 | 31.046 | 1.00 | 46.67 |
| | ATOM | 1972 | C | SER | B | 309 | 19.072 | 19.028 | 30.529 | 1.00 | 42.60 |
| | ATOM | 1973 | O | SER | B | 309 | 20.053 | 19.119 | 31.269 | 1.00 | 44.18 |
| | ATOM | 1974 | N | LEU | B | 310 | 18.217 | 18.012 | 30.596 | 1.00 | 39.44 |
| 55 | ATOM | 1975 | CA | LEU | B | 310 | 18.394 | 16.936 | 31.569 | 1.00 | 37.62 |
| | ATOM | 1976 | CB | LEU | B | 310 | 17.205 | 15.969 | 31.499 | 1.00 | 38.84 |
| | ATOM | 1977 | CG | LEU | B | 310 | 16.216 | 15.873 | 32.668 | 1.00 | 42.43 |
| | ATOM | 1978 | CD1 | LEU | B | 310 | 16.040 | 17.219 | 33.355 | 1.00 | 42.55 |
| | ATOM | 1979 | CD2 | LEU | B | 310 | 14.881 | 15.380 | 32.138 | 1.00 | 39.69 |
| 60 | ATOM | 1980 | C | LEU | B | 310 | 19.691 | 16.174 | 31.285 | 1.00 | 34.11 |
| | ATOM | 1981 | O | LEU | B | 310 | 20.111 | 16.070 | 30.139 | 1.00 | 34.41 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1982 | N | THR | B | 311 | 20.339 | 15.662 | 32.326 | 1.00 | 34.04 |
| | ATOM | 1983 | CA | THR | B | 311 | 21.564 | 14.888 | 32.127 | 1.00 | 32.34 |
| | ATOM | 1984 | CB | THR | B | 311 | 22.434 | 14.824 | 33.399 | 1.00 | 31.75 |
| | ATOM | 1985 | OG1 | THR | B | 311 | 21.724 | 14.116 | 34.420 | 1.00 | 36.20 |
| | ATOM | 1986 | CG2 | THR | B | 311 | 22.782 | 16.212 | 33.893 | 1.00 | 31.05 |
| 10 | ATOM | 1987 | C | THR | B | 311 | 21.145 | 13.460 | 31.790 | 1.00 | 32.37 |
| | ATOM | 1988 | O | THR | B | 311 | 19.967 | 13.117 | 31.899 | 1.00 | 28.16 |
| | ATOM | 1989 | N | ALA | B | 312 | 22.106 | 12.628 | 31.396 | 1.00 | 33.23 |
| | ATOM | 1990 | CA | ALA | B | 312 | 21.811 | 11.237 | 31.053 | 1.00 | 35.63 |
| | ATOM | 1991 | CB | ALA | B | 312 | 23.077 | 10.527 | 30.577 | 1.00 | 34.00 |
| 15 | ATOM | 1992 | C | ALA | B | 312 | 21.210 | 10.489 | 32.240 | 1.00 | 34.29 |
| | ATOM | 1993 | O | ALA | B | 312 | 20.226 | 9.766 | 32.089 | 1.00 | 33.10 |
| | ATOM | 1994 | N | ASP | B | 313 | 21.800 | 10.665 | 33.419 | 1.00 | 33.90 |
| | ATOM | 1995 | CA | ASP | B | 313 | 21.304 | 9.994 | 34.615 | 1.00 | 34.19 |
| | ATOM | 1996 | CB | ASP | B | 313 | 22.258 | 10.219 | 35.788 | 1.00 | 42.09 |
| 20 | ATOM | 1997 | CG | ASP | B | 313 | 23.494 | 9.358 | 35.700 | 1.00 | 44.87 |
| | ATOM | 1998 | OD1 | ASP | B | 313 | 24.586 | 9.858 | 36.040 | 1.00 | 51.57 |
| | ATOM | 1999 | OD2 | ASP | B | 313 | 23.377 | 8.184 | 35.290 | 1.00 | 46.79 |
| | ATOM | 2000 | C | ASP | B | 313 | 19.925 | 10.520 | 34.971 | 1.00 | 31.99 |
| | ATOM | 2001 | O | ASP | B | 313 | 19.056 | 9.768 | 35.426 | 1.00 | 32.03 |
| 25 | ATOM | 2002 | N | GLN | B | 314 | 19.733 | 11.819 | 34.763 | 1.00 | 29.38 |
| | ATOM | 2003 | CA | GLN | B | 314 | 18.458 | 12.457 | 35.046 | 1.00 | 29.73 |
| | ATOM | 2004 | CB | GLN | B | 314 | 18.562 | 13.966 | 34.832 | 1.00 | 32.88 |
| | ATOM | 2005 | CG | GLN | B | 314 | 18.970 | 14.732 | 36.085 | 1.00 | 36.47 |
| | ATOM | 2006 | CD | GLN | B | 314 | 19.213 | 16.208 | 35.815 | 1.00 | 36.76 |
| 30 | ATOM | 2007 | OE1 | GLN | B | 314 | 19.300 | 16.634 | 34.664 | 1.00 | 38.79 |
| | ATOM | 2008 | NE2 | GLN | B | 314 | 19.327 | 16.995 | 36.880 | 1.00 | 39.72 |
| | ATOM | 2009 | C | GLN | B | 314 | 17.409 | 11.873 | 34.116 | 1.00 | 29.11 |
| | ATOM | 2010 | O | GLN | B | 314 | 16.274 | 11.620 | 34.522 | 1.00 | 28.82 |
| | ATOM | 2011 | N | MET | B | 315 | 17.801 | 11.657 | 32.864 | 1.00 | 27.27 |
| 35 | ATOM | 2012 | CA | MET | B | 315 | 16.900 | 11.079 | 31.872 | 1.00 | 30.41 |
| | ATOM | 2013 | CB | MET | B | 315 | 17.595 | 11.029 | 30.509 | 1.00 | 30.10 |
| | ATOM | 2014 | CG | MET | B | 315 | 16.787 | 10.345 | 29.421 | 1.00 | 38.02 |
| | ATOM | 2015 | SD | MET | B | 315 | 15.252 | 11.220 | 29.065 | 1.00 | 41.12 |
| | ATOM | 2016 | CE | MET | B | 315 | 15.890 | 12.835 | 28.611 | 1.00 | 39.32 |
| 40 | ATOM | 2017 | C | MET | B | 315 | 16.490 | 9.665 | 32.311 | 1.00 | 27.99 |
| | ATOM | 2018 | O | MET | B | 315 | 15.302 | 9.351 | 32.396 | 1.00 | 26.60 |
| | ATOM | 2019 | N | VAL | B | 316 | 17.481 | 8.823 | 32.598 | 1.00 | 27.26 |
| | ATOM | 2020 | CA | VAL | B | 316 | 17.229 | 7.447 | 33.027 | 1.00 | 24.54 |
| | ATOM | 2021 | CB | VAL | B | 316 | 18.554 | 6.708 | 33.351 | 1.00 | 26.22 |
| 45 | ATOM | 2022 | CG1 | VAL | B | 316 | 18.272 | 5.404 | 34.096 | 1.00 | 29.81 |
| | ATOM | 2023 | CG2 | VAL | B | 316 | 19.302 | 6.410 | 32.074 | 1.00 | 29.75 |
| | ATOM | 2024 | C | VAL | B | 316 | 16.326 | 7.389 | 34.258 | 1.00 | 27.22 |
| | ATOM | 2025 | O | VAL | B | 316 | 15.397 | 6.579 | 34.318 | 1.00 | 25.55 |
| | ATOM | 2026 | N | SER | B | 317 | 16.601 | 8.243 | 35.242 | 1.00 | 24.40 |
| 50 | ATOM | 2027 | CA | SER | B | 317 | 15.799 | 8.268 | 36.460 | 1.00 | 27.63 |
| | ATOM | 2028 | CB | SER | B | 317 | 16.358 | 9.294 | 37.451 | 1.00 | 31.68 |
| | ATOM | 2029 | OG | SER | B | 317 | 17.492 | 8.771 | 38.112 | 1.00 | 39.97 |
| | ATOM | 2030 | C | SER | B | 317 | 14.346 | 8.600 | 36.154 | 1.00 | 26.73 |
| | ATOM | 2031 | O | SER | B | 317 | 13.434 | 7.932 | 36.648 | 1.00 | 25.65 |
| 55 | ATOM | 2032 | N | ALA | B | 318 | 14.135 | 9.634 | 35.342 | 1.00 | 24.19 |
| | ATOM | 2033 | CA | ALA | B | 318 | 12.786 | 10.049 | 34.969 | 1.00 | 24.17 |
| | ATOM | 2034 | CB | ALA | B | 318 | 12.850 | 11.250 | 34.022 | 1.00 | 21.44 |
| | ATOM | 2035 | C | ALA | B | 318 | 12.038 | 8.890 | 34.306 | 1.00 | 21.63 |
| | ATOM | 2036 | O | ALA | B | 318 | 10.902 | 8.598 | 34.648 | 1.00 | 20.25 |
| 60 | ATOM | 2037 | N | LEU | B | 319 | 12.695 | 8.225 | 33.364 | 1.00 | 23.37 |
| | ATOM | 2038 | CA | LEU | B | 319 | 12.098 | 7.102 | 32.652 | 1.00 | 25.42 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 2039 | CB | LEU | B | 319 | 13.050 | 6.635 | 31.548 | 1.00 | 22.03 |
| | ATOM | 2040 | CG | LEU | B | 319 | 13.264 | 7.622 | 30.394 | 1.00 | 20.71 |
| | ATOM | 2041 | CD1 | LEU | B | 319 | 14.146 | 6.995 | 29.331 | 1.00 | 23.60 |
| | ATOM | 2042 | CD2 | LEU | B | 319 | 11.918 | 8.020 | 29.803 | 1.00 | 23.82 |
| | ATOM | 2043 | C | LEU | B | 319 | 11.729 | 5.926 | 33.564 | 1.00 | 27.26 |
| 10 | ATOM | 2044 | O | LEU | B | 319 | 10.615 | 5.396 | 33.488 | 1.00 | 28.91 |
| | ATOM | 2045 | N | LEU | B | 320 | 12.656 | 5.516 | 34.426 | 1.00 | 26.58 |
| | ATOM | 2046 | CA | LEU | B | 320 | 12.399 | 4.405 | 35.334 | 1.00 | 26.73 |
| | ATOM | 2047 | CB | LEU | B | 320 | 13.657 | 4.075 | 36.145 | 1.00 | 26.87 |
| | ATOM | 2048 | CG | LEU | B | 320 | 14.846 | 3.460 | 35.398 | 1.00 | 26.15 |
| 15 | ATOM | 2049 | CD1 | LEU | B | 320 | 16.053 | 3.375 | 36.330 | 1.00 | 28.04 |
| | ATOM | 2050 | CD2 | LEU | B | 320 | 14.484 | 2.076 | 34.895 | 1.00 | 26.96 |
| | ATOM | 2051 | C | LEU | B | 320 | 11.249 | 4.722 | 36.290 | 1.00 | 29.19 |
| | ATOM | 2052 | O | LEU | B | 320 | 10.449 | 3.849 | 36.631 | 1.00 | 26.66 |
| | ATOM | 2053 | N | ASP | B | 321 | 11.160 | 5.976 | 36.719 | 1.00 | 29.72 |
| 20 | ATOM | 2054 | CA | ASP | B | 321 | 10.112 | 6.371 | 37.647 | 1.00 | 31.36 |
| | ATOM | 2055 | CB | ASP | B | 321 | 10.494 | 7.683 | 38.336 | 1.00 | 36.60 |
| | ATOM | 2056 | CG | ASP | B | 321 | 11.407 | 7.461 | 39.535 | 1.00 | 46.11 |
| | ATOM | 2057 | OD1 | ASP | B | 321 | 10.897 | 7.058 | 40.605 | 1.00 | 46.64 |
| | ATOM | 2058 | OD2 | ASP | B | 321 | 12.635 | 7.676 | 39.402 | 1.00 | 45.98 |
| 25 | ATOM | 2059 | C | ASP | B | 321 | 8.742 | 6.494 | 36.989 | 1.00 | 28.29 |
| | ATOM | 2060 | O | ASP | B | 321 | 7.715 | 6.432 | 37.661 | 1.00 | 27.19 |
| | ATOM | 2061 | N | ALA | B | 322 | 8.726 | 6.650 | 35.672 | 1.00 | 28.34 |
| | ATOM | 2062 | CA | ALA | B | 322 | 7.469 | 6.779 | 34.950 | 1.00 | 25.55 |
| | ATOM | 2063 | CB | ALA | B | 322 | 7.668 | 7.668 | 33.728 | 1.00 | 24.11 |
| 30 | ATOM | 2064 | C | ALA | B | 322 | 6.911 | 5.420 | 34.523 | 1.00 | 22.80 |
| | ATOM | 2065 | O | ALA | B | 322 | 5.810 | 5.338 | 33.979 | 1.00 | 24.54 |
| | ATOM | 2066 | N | GLU | B | 323 | 7.662 | 4.355 | 34.781 | 1.00 | 20.16 |
| | ATOM | 2067 | CA | GLU | B | 323 | 7.229 | 3.021 | 34.386 | 1.00 | 21.44 |
| | ATOM | 2068 | CB | GLU | B | 323 | 8.196 | 1.982 | 34.938 | 1.00 | 23.72 |
| 35 | ATOM | 2069 | CG | GLU | B | 323 | 9.393 | 1.746 | 34.024 | 1.00 | 23.58 |
| | ATOM | 2070 | CD | GLU | B | 323 | 8.988 | 1.134 | 32.685 | 1.00 | 25.23 |
| | ATOM | 2071 | OE1 | GLU | B | 323 | 8.852 | 1.881 | 31.692 | 1.00 | 21.74 |
| | ATOM | 2072 | OE2 | GLU | B | 323 | 8.809 | -0.095 | 32.624 | 1.00 | 25.49 |
| | ATOM | 2073 | C | GLU | B | 323 | 5.796 | 2.696 | 34.810 | 1.00 | 22.35 |
| 40 | ATOM | 2074 | O | GLU | B | 323 | 5.409 | 2.926 | 35.951 | 1.00 | 22.34 |
| | ATOM | 2075 | N | PRO | B | 324 | 4.986 | 2.165 | 33.880 | 1.00 | 19.10 |
| | ATOM | 2076 | CD | PRO | B | 324 | 5.286 | 1.806 | 32.483 | 1.00 | 19.11 |
| | ATOM | 2077 | CA | PRO | B | 324 | 3.607 | 1.839 | 34.242 | 1.00 | 22.04 |
| | ATOM | 2078 | CB | PRO | B | 324 | 2.919 | 1.658 | 32.893 | 1.00 | 21.96 |
| 45 | ATOM | 2079 | CG | PRO | B | 324 | 4.015 | 1.137 | 32.015 | 1.00 | 24.13 |
| | ATOM | 2080 | C | PRO | B | 324 | 3.619 | 0.556 | 35.060 | 1.00 | 23.44 |
| | ATOM | 2081 | O | PRO | B | 324 | 4.590 | -0.200 | 35.028 | 1.00 | 22.20 |
| | ATOM | 2082 | N | PRO | B | 325 | 2.540 | 0.287 | 35.801 | 1.00 | 24.88 |
| | ATOM | 2083 | CD | PRO | B | 325 | 1.299 | 1.068 | 35.945 | 1.00 | 26.67 |
| 50 | ATOM | 2084 | CA | PRO | B | 325 | 2.520 | -0.940 | 36.603 | 1.00 | 25.10 |
| | ATOM | 2085 | CB | PRO | B | 325 | 1.394 | -0.691 | 37.595 | 1.00 | 27.09 |
| | ATOM | 2086 | CG | PRO | B | 325 | 0.448 | 0.205 | 36.854 | 1.00 | 26.87 |
| | ATOM | 2087 | C | PRO | B | 325 | 2.270 | -2.192 | 35.776 | 1.00 | 25.77 |
| | ATOM | 2088 | O | PRO | B | 325 | 1.853 | -2.118 | 34.617 | 1.00 | 21.69 |
| 55 | ATOM | 2089 | N | ILE | B | 326 | 2.538 | -3.344 | 36.379 | 1.00 | 24.05 |
| | ATOM | 2090 | CA | ILE | B | 326 | 2.301 | -4.620 | 35.722 | 1.00 | 22.51 |
| | ATOM | 2091 | CB | ILE | B | 326 | 3.303 | -5.688 | 36.185 | 1.00 | 25.81 |
| | ATOM | 2092 | CG2 | ILE | B | 326 | 3.011 | -7.018 | 35.481 | 1.00 | 23.78 |
| | ATOM | 2093 | CG1 | ILE | B | 326 | 4.729 | -5.209 | 35.900 | 1.00 | 25.75 |
| 60 | ATOM | 2094 | CD1 | ILE | B | 326 | 5.241 | -5.585 | 34.533 | 1.00 | 27.78 |
| | ATOM | 2095 | C | ILE | B | 326 | 0.893 | -5.020 | 36.149 | 1.00 | 23.63 |

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|----|------|------|-----|-----|---|-----|---------|---------|--------|------|-------|
| 5 | ATOM | 2096 | O | ILE | B | 326 | 0.632 | -5.231 | 37.332 | 1.00 | 24.81 |
| | ATOM | 2097 | N | LEU | B | 327 | -0.018 | -5.104 | 35.188 | 1.00 | 19.44 |
| | ATOM | 2098 | CA | LEU | B | 327 | -1.399 | -5.437 | 35.493 | 1.00 | 17.03 |
| | ATOM | 2099 | CB | LEU | B | 327 | -2.336 | -4.747 | 34.493 | 1.00 | 18.39 |
| | ATOM | 2100 | CG | LEU | B | 327 | -2.201 | -3.216 | 34.373 | 1.00 | 20.69 |
| 10 | ATOM | 2101 | CD1 | LEU | B | 327 | -3.245 | -2.679 | 33.406 | 1.00 | 14.87 |
| | ATOM | 2102 | CD2 | LEU | B | 327 | -2.384 | -2.570 | 35.742 | 1.00 | 14.39 |
| | ATOM | 2103 | C | LEU | B | 327 | -1.662 | -6.928 | 35.499 | 1.00 | 19.87 |
| | ATOM | 2104 | O | LEU | B | 327 | -0.854 | -7.722 | 35.014 | 1.00 | 20.90 |
| | ATOM | 2105 | N | TYR | B | 328 | -2.803 | -7.300 | 36.066 | 1.00 | 20.92 |
| 15 | ATOM | 2106 | CA | TYR | B | 328 | -3.202 | -8.692 | 36.135 | 1.00 | 21.79 |
| | ATOM | 2107 | CB | TYR | B | 328 | -3.658 | -9.050 | 37.550 | 1.00 | 22.91 |
| | ATOM | 2108 | CG | TYR | B | 328 | -2.515 | -9.376 | 38.468 | 1.00 | 24.60 |
| | ATOM | 2109 | CD1 | TYR | B | 328 | -2.118 | -10.696 | 38.677 | 1.00 | 25.93 |
| | ATOM | 2110 | CE1 | TYR | B | 328 | -1.034 | -11.000 | 39.498 | 1.00 | 28.10 |
| 20 | ATOM | 2111 | CD2 | TYR | B | 328 | -1.802 | -8.362 | 39.103 | 1.00 | 29.46 |
| | ATOM | 2112 | CE2 | TYR | B | 328 | -0.716 | -8.654 | 39.926 | 1.00 | 35.30 |
| | ATOM | 2113 | CZ | TYR | B | 328 | -0.338 | -9.973 | 40.117 | 1.00 | 32.59 |
| | ATOM | 2114 | OH | TYR | B | 328 | 0.739 | -10.257 | 40.923 | 1.00 | 37.24 |
| | ATOM | 2115 | C | TYR | B | 328 | -4.336 | -8.944 | 35.168 | 1.00 | 22.25 |
| 25 | ATOM | 2116 | O | TYR | B | 328 | -5.115 | -8.039 | 34.849 | 1.00 | 19.77 |
| | ATOM | 2117 | N | SER | B | 329 | -4.420 | -10.180 | 34.698 | 1.00 | 25.81 |
| | ATOM | 2118 | CA | SER | B | 329 | -5.480 | -10.571 | 33.787 | 1.00 | 29.39 |
| | ATOM | 2119 | CB | SER | B | 329 | -5.002 | -11.710 | 32.887 | 1.00 | 27.65 |
| | ATOM | 2120 | OG | SER | B | 329 | -6.091 | -12.329 | 32.233 | 1.00 | 28.98 |
| 30 | ATOM | 2121 | C | SER | B | 329 | -6.625 | -11.042 | 34.673 | 1.00 | 33.17 |
| | ATOM | 2122 | O | SER | B | 329 | -6.453 | -11.157 | 35.888 | 1.00 | 32.52 |
| | ATOM | 2123 | N | GLU | B | 330 | -7.792 | -11.289 | 34.084 | 1.00 | 38.75 |
| | ATOM | 2124 | CA | GLU | B | 330 | -8.930 | -11.776 | 34.859 | 1.00 | 44.91 |
| | ATOM | 2125 | CB | GLU | B | 330 | -10.134 | -11.999 | 33.951 | 1.00 | 45.63 |
| 35 | ATOM | 2126 | C | GLU | B | 330 | -8.493 | -13.093 | 35.491 | 1.00 | 48.62 |
| | ATOM | 2127 | O | GLU | B | 330 | -7.739 | -13.851 | 34.882 | 1.00 | 52.37 |
| | ATOM | 2128 | N | TYR | B | 331 | -8.952 | -13.366 | 36.707 | 1.00 | 51.75 |
| | ATOM | 2129 | CA | TYR | B | 331 | -8.575 | -14.596 | 37.396 | 1.00 | 55.25 |
| | ATOM | 2130 | CB | TYR | B | 331 | -8.538 | -14.365 | 38.911 | 1.00 | 53.04 |
| 40 | ATOM | 2131 | CG | TYR | B | 331 | -9.769 | -13.668 | 39.440 | 1.00 | 50.70 |
| | ATOM | 2132 | CD1 | TYR | B | 331 | -10.880 | -14.400 | 39.856 | 1.00 | 47.09 |
| | ATOM | 2133 | CE1 | TYR | B | 331 | -12.035 | -13.762 | 40.292 | 1.00 | 46.43 |
| | ATOM | 2134 | CD2 | TYR | B | 331 | -9.842 | -12.273 | 39.478 | 1.00 | 47.52 |
| | ATOM | 2135 | CE2 | TYR | B | 331 | -10.993 | -11.625 | 39.913 | 1.00 | 43.98 |
| 45 | ATOM | 2136 | CZ | TYR | B | 331 | -12.086 | -12.376 | 40.314 | 1.00 | 44.33 |
| | ATOM | 2137 | OH | TYR | B | 331 | -13.239 | -11.747 | 40.715 | 1.00 | 45.31 |
| | ATOM | 2138 | C | TYR | B | 331 | -9.528 | -15.743 | 37.075 | 1.00 | 60.11 |
| | ATOM | 2139 | O | TYR | B | 331 | -10.748 | -15.569 | 37.066 | 1.00 | 63.13 |
| | ATOM | 2140 | N | ASP | B | 332 | -8.952 | -16.913 | 36.809 | 1.00 | 61.60 |
| 50 | ATOM | 2141 | CA | ASP | B | 332 | -9.704 | -18.124 | 36.490 | 1.00 | 63.58 |
| | ATOM | 2142 | CB | ASP | B | 332 | -10.637 | -17.895 | 35.298 | 1.00 | 65.11 |
| | ATOM | 2143 | CG | ASP | B | 332 | -11.723 | -18.953 | 35.200 | 1.00 | 65.32 |
| | ATOM | 2144 | OD1 | ASP | B | 332 | -11.420 | -20.136 | 35.463 | 1.00 | 63.69 |
| | ATOM | 2145 | OD2 | ASP | B | 332 | -12.876 | -18.602 | 34.866 | 1.00 | 63.61 |
| 55 | ATOM | 2146 | C | ASP | B | 332 | -8.707 | -19.227 | 36.153 | 1.00 | 62.86 |
| | ATOM | 2147 | O | ASP | B | 332 | -7.853 | -19.056 | 35.287 | 1.00 | 62.26 |
| | ATOM | 2148 | N | PRO | B | 333 | -8.811 | -20.379 | 36.833 | 1.00 | 63.96 |
| | ATOM | 2149 | CD | PRO | B | 333 | -9.808 | -20.690 | 37.875 | 1.00 | 64.24 |
| | ATOM | 2150 | CA | PRO | B | 333 | -7.901 | -21.503 | 36.596 | 1.00 | 64.24 |
| 60 | ATOM | 2151 | CB | PRO | B | 333 | -8.015 | -22.325 | 37.874 | 1.00 | 64.70 |
| | ATOM | 2152 | CG | PRO | B | 333 | -9.410 | -22.071 | 38.347 | 1.00 | 65.00 |

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|----|------|------|-----|-----|---|-----|---------|---------|--------|------|-------|
| 5 | ATOM | 2153 | C | PRO | B | 333 | -8.180 | -22.340 | 35.351 | 1.00 | 63.90 |
| | ATOM | 2154 | O | PRO | B | 333 | -7.384 | -23.214 | 35.007 | 1.00 | 63.70 |
| | ATOM | 2155 | N | THR | B | 334 | -9.303 | -22.084 | 34.683 | 1.00 | 63.83 |
| | ATOM | 2156 | CA | THR | B | 334 | -9.649 | -22.832 | 33.475 | 1.00 | 63.77 |
| | ATOM | 2157 | CB | THR | B | 334 | -11.065 | -22.477 | 32.975 | 1.00 | 64.63 |
| 10 | ATOM | 2158 | OG1 | THR | B | 334 | -11.132 | -21.078 | 32.675 | 1.00 | 65.95 |
| | ATOM | 2159 | CG2 | THR | B | 334 | -12.102 | -22.817 | 34.036 | 1.00 | 65.09 |
| | ATOM | 2160 | C | THR | B | 334 | -8.634 | -22.499 | 32.388 | 1.00 | 62.62 |
| | ATOM | 2161 | O | THR | B | 334 | -8.931 | -21.774 | 31.437 | 1.00 | 60.15 |
| | ATOM | 2162 | N | ARG | B | 335 | -7.432 | -23.043 | 32.553 | 1.00 | 63.14 |
| 15 | ATOM | 2163 | CA | ARG | B | 335 | -6.324 | -22.820 | 31.633 | 1.00 | 60.70 |
| | ATOM | 2164 | CB | ARG | B | 335 | -5.130 | -23.667 | 32.050 | 1.00 | 58.73 |
| | ATOM | 2165 | C | ARG | B | 335 | -6.667 | -23.086 | 30.174 | 1.00 | 59.71 |
| | ATOM | 2166 | O | ARG | B | 335 | -6.302 | -22.298 | 29.298 | 1.00 | 62.33 |
| | ATOM | 2167 | N | PRO | B | 336 | -7.377 | -24.194 | 29.884 | 1.00 | 55.25 |
| 20 | ATOM | 2168 | CD | PRO | B | 336 | -7.938 | -25.227 | 30.769 | 1.00 | 53.53 |
| | ATOM | 2169 | CA | PRO | B | 336 | -7.698 | -24.437 | 28.471 | 1.00 | 50.10 |
| | ATOM | 2170 | CB | PRO | B | 336 | -8.399 | -25.799 | 28.476 | 1.00 | 49.70 |
| | ATOM | 2171 | CG | PRO | B | 336 | -8.164 | -26.372 | 29.844 | 1.00 | 50.71 |
| | ATOM | 2172 | C | PRO | B | 336 | -8.602 | -23.324 | 27.954 | 1.00 | 44.54 |
| 25 | ATOM | 2173 | O | PRO | B | 336 | -9.809 | -23.342 | 28.179 | 1.00 | 44.14 |
| | ATOM | 2174 | N | PHE | B | 337 | -8.007 | -22.350 | 27.274 | 1.00 | 39.18 |
| | ATOM | 2175 | CA | PHE | B | 337 | -8.764 | -21.223 | 26.742 | 1.00 | 38.25 |
| | ATOM | 2176 | CB | PHE | B | 337 | -7.850 | -20.003 | 26.567 | 1.00 | 36.98 |
| | ATOM | 2177 | CG | PHE | B | 337 | -7.229 | -19.517 | 27.846 | 1.00 | 36.81 |
| 30 | ATOM | 2178 | CD1 | PHE | B | 337 | -5.846 | -19.511 | 28.002 | 1.00 | 38.89 |
| | ATOM | 2179 | CD2 | PHE | B | 337 | -8.023 | -19.062 | 28.893 | 1.00 | 35.97 |
| | ATOM | 2180 | CE1 | PHE | B | 337 | -5.262 | -19.059 | 29.185 | 1.00 | 36.85 |
| | ATOM | 2181 | CE2 | PHE | B | 337 | -7.449 | -18.608 | 30.079 | 1.00 | 37.15 |
| | ATOM | 2182 | CZ | PHE | B | 337 | -6.064 | -18.607 | 30.224 | 1.00 | 38.40 |
| 35 | ATOM | 2183 | C | PHE | B | 337 | -9.420 | -21.535 | 25.402 | 1.00 | 36.81 |
| | ATOM | 2184 | O | PHE | B | 337 | -8.962 | -22.399 | 24.658 | 1.00 | 36.26 |
| | ATOM | 2185 | N | SER | B | 338 | -10.504 | -20.828 | 25.107 | 1.00 | 35.85 |
| | ATOM | 2186 | CA | SER | B | 338 | -11.198 | -20.981 | 23.836 | 1.00 | 34.76 |
| | ATOM | 2187 | CB | SER | B | 338 | -12.713 | -20.948 | 24.035 | 1.00 | 34.85 |
| 40 | ATOM | 2188 | OG | SER | B | 338 | -13.164 | -19.621 | 24.235 | 1.00 | 33.53 |
| | ATOM | 2189 | C | SER | B | 338 | -10.761 | -19.761 | 23.037 | 1.00 | 34.99 |
| | ATOM | 2190 | O | SER | B | 338 | -10.143 | -18.855 | 23.591 | 1.00 | 34.32 |
| | ATOM | 2191 | N | GLU | B | 339 | -11.075 | -19.722 | 21.750 | 1.00 | 33.01 |
| | ATOM | 2192 | CA | GLU | B | 339 | -10.682 | -18.579 | 20.950 | 1.00 | 33.94 |
| 45 | ATOM | 2193 | CB | GLU | B | 339 | -11.146 | -18.737 | 19.501 | 1.00 | 33.79 |
| | ATOM | 2194 | CG | GLU | B | 339 | -10.758 | -17.553 | 18.623 | 1.00 | 39.11 |
| | ATOM | 2195 | CD | GLU | B | 339 | -10.865 | -17.852 | 17.137 | 1.00 | 43.17 |
| | ATOM | 2196 | OE1 | GLU | B | 339 | -11.990 | -17.785 | 16.600 | 1.00 | 45.28 |
| | ATOM | 2197 | OE2 | GLU | B | 339 | -9.824 | -18.152 | 16.510 | 1.00 | 39.19 |
| 50 | ATOM | 2198 | C | GLU | B | 339 | -11.265 | -17.295 | 21.531 | 1.00 | 34.28 |
| | ATOM | 2199 | O | GLU | B | 339 | -10.575 | -16.283 | 21.631 | 1.00 | 33.65 |
| | ATOM | 2200 | N | ALA | B | 340 | -12.535 | -17.339 | 21.920 | 1.00 | 31.12 |
| | ATOM | 2201 | CA | ALA | B | 340 | -13.194 | -16.164 | 22.469 | 1.00 | 29.10 |
| | ATOM | 2202 | CB | ALA | B | 340 | -14.696 | -16.412 | 22.573 | 1.00 | 33.84 |
| 55 | ATOM | 2203 | C | ALA | B | 340 | -12.639 | -15.731 | 23.826 | 1.00 | 28.98 |
| | ATOM | 2204 | O | ALA | B | 340 | -12.431 | -14.541 | 24.060 | 1.00 | 30.48 |
| | ATOM | 2205 | N | SER | B | 341 | -12.407 | -16.691 | 24.719 | 1.00 | 26.66 |
| | ATOM | 2206 | CA | SER | B | 341 | -11.882 | -16.386 | 26.044 | 1.00 | 24.26 |
| | ATOM | 2207 | CB | SER | B | 341 | -11.867 | -17.643 | 26.923 | 1.00 | 27.04 |
| 60 | ATOM | 2208 | OG | SER | B | 341 | -10.851 | -18.541 | 26.515 | 1.00 | 33.84 |
| | ATOM | 2209 | C | SER | B | 341 | -10.479 | -15.793 | 25.960 | 1.00 | 23.97 |

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|----|------|------|-----|-----|---|-----|---------|---------|--------|------|-------|
| 5 | ATOM | 2210 | O | SER | B | 341 | -10.171 | -14.824 | 26.651 | 1.00 | 21.56 |
| | ATOM | 2211 | N | MET | B | 342 | -9.631 | -16.368 | 25.114 | 1.00 | 26.83 |
| | ATOM | 2212 | CA | MET | B | 342 | -8.271 | -15.865 | 24.954 | 1.00 | 27.24 |
| | ATOM | 2213 | CB | MET | B | 342 | -7.477 | -16.758 | 24.001 | 1.00 | 30.45 |
| | ATOM | 2214 | CG | MET | B | 342 | -6.038 | -16.300 | 23.802 | 1.00 | 35.35 |
| 10 | ATOM | 2215 | SD | MET | B | 342 | -4.866 | -17.667 | 23.777 | 1.00 | 44.57 |
| | ATOM | 2216 | CE | MET | B | 342 | -4.034 | -17.341 | 22.244 | 1.00 | 41.37 |
| | ATOM | 2217 | C | MET | B | 342 | -8.322 | -14.448 | 24.385 | 1.00 | 25.31 |
| | ATOM | 2218 | O | MET | B | 342 | -7.653 | -13.541 | 24.874 | 1.00 | 26.67 |
| | ATOM | 2219 | N | MET | B | 343 | -9.114 | -14.278 | 23.345 | 1.00 | 25.75 |
| 15 | ATOM | 2220 | CA | MET | B | 343 | -9.262 | -12.979 | 22.712 | 1.00 | 25.47 |
| | ATOM | 2221 | CB | MET | B | 343 | -10.210 | -13.088 | 21.528 | 1.00 | 23.51 |
| | ATOM | 2222 | CG | MET | B | 343 | -9.540 | -13.618 | 20.273 | 1.00 | 28.86 |
| | ATOM | 2223 | SD | MET | B | 343 | -8.325 | -12.456 | 19.609 | 1.00 | 29.25 |
| | ATOM | 2224 | CE | MET | B | 343 | -9.344 | -11.015 | 19.371 | 1.00 | 28.74 |
| 20 | ATOM | 2225 | C | MET | B | 343 | -9.798 | -11.966 | 23.712 | 1.00 | 25.37 |
| | ATOM | 2226 | O | MET | B | 343 | -9.360 | -10.810 | 23.728 | 1.00 | 24.98 |
| | ATOM | 2227 | N | GLY | B | 344 | -10.739 | -12.403 | 24.536 | 1.00 | 23.91 |
| | ATOM | 2228 | CA | GLY | B | 344 | -11.320 | -11.526 | 25.536 | 1.00 | 22.43 |
| | ATOM | 2229 | C | GLY | B | 344 | -10.313 | -11.103 | 26.592 | 1.00 | 22.06 |
| 25 | ATOM | 2230 | O | GLY | B | 344 | -10.262 | -9.934 | 26.982 | 1.00 | 20.87 |
| | ATOM | 2231 | N | LEU | B | 345 | -9.511 | -12.048 | 27.063 | 1.00 | 19.36 |
| | ATOM | 2232 | CA | LEU | B | 345 | -8.520 | -11.748 | 28.083 | 1.00 | 25.74 |
| | ATOM | 2233 | CB | LEU | B | 345 | -7.886 | -13.040 | 28.600 | 1.00 | 26.78 |
| | ATOM | 2234 | CG | LEU | B | 345 | -8.794 | -14.010 | 29.362 | 1.00 | 30.04 |
| 30 | ATOM | 2235 | CD1 | LEU | B | 345 | -8.099 | -15.357 | 29.488 | 1.00 | 28.39 |
| | ATOM | 2236 | CD2 | LEU | B | 345 | -9.122 | -13.443 | 30.736 | 1.00 | 29.93 |
| | ATOM | 2237 | C | LEU | B | 345 | -7.425 | -10.822 | 27.550 | 1.00 | 23.24 |
| | ATOM | 2238 | O | LEU | B | 345 | -7.037 | -9.865 | 28.212 | 1.00 | 23.43 |
| | ATOM | 2239 | N | LEU | B | 346 | -6.937 | -11.108 | 26.350 | 1.00 | 21.92 |
| 35 | ATOM | 2240 | CA | LEU | B | 346 | -5.874 | -10.303 | 25.763 | 1.00 | 22.71 |
| | ATOM | 2241 | CB | LEU | B | 346 | -5.343 | -10.962 | 24.486 | 1.00 | 23.17 |
| | ATOM | 2242 | CG | LEU | B | 346 | -4.684 | -12.331 | 24.668 | 1.00 | 20.66 |
| | ATOM | 2243 | CD1 | LEU | B | 346 | -4.303 | -12.916 | 23.309 | 1.00 | 18.75 |
| | ATOM | 2244 | CD2 | LEU | B | 346 | -3.464 | -12.188 | 25.553 | 1.00 | 20.84 |
| 40 | ATOM | 2245 | C | LEU | B | 346 | -6.304 | -8.873 | 25.458 | 1.00 | 22.99 |
| | ATOM | 2246 | O | LEU | B | 346 | -5.540 | -7.935 | 25.695 | 1.00 | 22.07 |
| | ATOM | 2247 | N | THR | B | 347 | -7.516 | -8.699 | 24.937 | 1.00 | 20.53 |
| | ATOM | 2248 | CA | THR | B | 347 | -7.987 | -7.357 | 24.608 | 1.00 | 21.89 |
| | ATOM | 2249 | CB | THR | B | 347 | -9.152 | -7.388 | 23.601 | 1.00 | 21.65 |
| 45 | ATOM | 2250 | OG1 | THR | B | 347 | -10.218 | -8.190 | 24.123 | 1.00 | 19.65 |
| | ATOM | 2251 | CG2 | THR | B | 347 | -8.676 | -7.955 | 22.262 | 1.00 | 22.01 |
| | ATOM | 2252 | C | THR | B | 347 | -8.426 | -6.590 | 25.853 | 1.00 | 23.60 |
| | ATOM | 2253 | O | THR | B | 347 | -8.358 | -5.357 | 25.883 | 1.00 | 20.31 |
| | ATOM | 2254 | N | ASN | B | 348 | -8.884 | -7.314 | 26.874 | 1.00 | 22.27 |
| 50 | ATOM | 2255 | CA | ASN | B | 348 | -9.293 | -6.667 | 28.114 | 1.00 | 23.99 |
| | ATOM | 2256 | CB | ASN | B | 348 | -10.008 | -7.642 | 29.056 | 1.00 | 22.32 |
| | ATOM | 2257 | CG | ASN | B | 348 | -10.342 | -7.022 | 30.398 | 1.00 | 28.26 |
| | ATOM | 2258 | OD1 | ASN | B | 348 | -9.478 | -6.746 | 31.216 | 1.00 | 27.14 |
| | ATOM | 2259 | ND2 | ASN | B | 348 | -11.647 | -6.764 | 30.625 | 1.00 | 27.02 |
| 55 | ATOM | 2260 | C | ASN | B | 348 | -8.035 | -6.120 | 28.798 | 1.00 | 19.48 |
| | ATOM | 2261 | O | ASN | B | 348 | -8.014 | -4.991 | 29.271 | 1.00 | 18.26 |
| | ATOM | 2262 | N | LEU | B | 349 | -6.984 | -6.931 | 28.832 | 1.00 | 19.07 |
| | ATOM | 2263 | CA | LEU | B | 349 | -5.724 | -6.516 | 29.446 | 1.00 | 20.37 |
| | ATOM | 2264 | CB | LEU | B | 349 | -4.716 | -7.674 | 29.434 | 1.00 | 18.21 |
| 60 | ATOM | 2265 | CG | LEU | B | 349 | -3.297 | -7.316 | 29.889 | 1.00 | 18.24 |
| | ATOM | 2266 | CD1 | LEU | B | 349 | -3.323 | -6.904 | 31.356 | 1.00 | 12.44 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|
| 5 | ATOM | 2267 | CD2 | LEU | B | 349 | -2.370 | -8.504 | 29.672 | 1.00 | 21.28 |
| | ATOM | 2268 | C | LEU | B | 349 | -5.131 | -5.307 | 28.718 | 1.00 | 19.92 |
| | ATOM | 2269 | O | LEU | B | 349 | -4.738 | -4.322 | 29.349 | 1.00 | 16.56 |
| | ATOM | 2270 | N | ALA | B | 350 | -5.067 | -5.391 | 27.391 | 1.00 | 16.67 |
| | ATOM | 2271 | CA | ALA | B | 350 | -4.529 | -4.308 | 26.578 | 1.00 | 17.11 |
| 10 | ATOM | 2272 | CB | ALA | B | 350 | -4.587 | -4.690 | 25.095 | 1.00 | 14.15 |
| | ATOM | 2273 | C | ALA | B | 350 | -5.272 | -2.988 | 26.805 | 1.00 | 17.92 |
| | ATOM | 2274 | O | ALA | B | 350 | -4.650 | -1.926 | 26.904 | 1.00 | 18.71 |
| | ATOM | 2275 | N | ASP | B | 351 | -6.600 | -3.053 | 26.857 | 1.00 | 17.51 |
| | ATOM | 2276 | CA | ASP | B | 351 | -7.409 | -1.856 | 27.074 | 1.00 | 16.57 |
| 15 | ATOM | 2277 | CB | ASP | B | 351 | -8.902 | -2.202 | 27.041 | 1.00 | 18.97 |
| | ATOM | 2278 | CG | ASP | B | 351 | -9.785 | -0.974 | 26.858 | 1.00 | 21.80 |
| | ATOM | 2279 | OD1 | ASP | B | 351 | -9.660 | -0.292 | 25.824 | 1.00 | 24.62 |
| | ATOM | 2280 | OD2 | ASP | B | 351 | -10.604 | -0.682 | 27.754 | 1.00 | 22.78 |
| | ATOM | 2281 | C | ASP | B | 351 | -7.064 | -1.228 | 28.415 | 1.00 | 16.81 |
| 20 | ATOM | 2282 | O | ASP | B | 351 | -6.963 | -0.009 | 28.534 | 1.00 | 15.75 |
| | ATOM | 2283 | N | ARG | B | 352 | -6.894 | -2.056 | 29.438 | 1.00 | 13.97 |
| | ATOM | 2284 | CA | ARG | B | 352 | -6.552 | -1.509 | 30.742 | 1.00 | 16.09 |
| | ATOM | 2285 | CB | ARG | B | 352 | -6.728 | -2.571 | 31.833 | 1.00 | 15.78 |
| | ATOM | 2286 | CG | ARG | B | 352 | -8.189 | -2.819 | 32.189 | 1.00 | 17.93 |
| 25 | ATOM | 2287 | CD | ARG | B | 352 | -8.323 | -3.882 | 33.279 | 1.00 | 19.84 |
| | ATOM | 2288 | NE | ARG | B | 352 | -8.010 | -5.222 | 32.785 | 1.00 | 21.36 |
| | ATOM | 2289 | CZ | ARG | B | 352 | -7.187 | -6.075 | 33.387 | 1.00 | 21.18 |
| | ATOM | 2290 | NH1 | ARG | B | 352 | -6.579 | -5.741 | 34.516 | 1.00 | 20.51 |
| | ATOM | 2291 | NH2 | ARG | B | 352 | -6.980 | -7.275 | 32.864 | 1.00 | 28.51 |
| 30 | ATOM | 2292 | C | ARG | B | 352 | -5.123 | -0.975 | 30.728 | 1.00 | 15.81 |
| | ATOM | 2293 | O | ARG | B | 352 | -4.835 | 0.057 | 31.339 | 1.00 | 15.61 |
| | ATOM | 2294 | N | GLU | B | 353 | -4.231 | -1.665 | 30.019 | 1.00 | 15.45 |
| | ATOM | 2295 | CA | GLU | B | 353 | -2.838 | -1.228 | 29.935 | 1.00 | 16.59 |
| | ATOM | 2296 | CB | GLU | B | 353 | -1.990 | -2.243 | 29.168 | 1.00 | 14.64 |
| 35 | ATOM | 2297 | CG | GLU | B | 353 | -1.554 | -3.456 | 29.973 | 1.00 | 18.23 |
| | ATOM | 2298 | CD | GLU | B | 353 | -0.620 | -4.355 | 29.176 | 1.00 | 22.72 |
| | ATOM | 2299 | OE1 | GLU | B | 353 | -1.099 | -5.078 | 28.275 | 1.00 | 21.94 |
| | ATOM | 2300 | OE2 | GLU | B | 353 | 0.599 | -4.324 | 29.442 | 1.00 | 24.41 |
| | ATOM | 2301 | C | GLU | B | 353 | -2.729 | 0.119 | 29.219 | 1.00 | 15.85 |
| 40 | ATOM | 2302 | O | GLU | B | 353 | -1.872 | 0.939 | 29.540 | 1.00 | 13.76 |
| | ATOM | 2303 | N | LEU | B | 354 | -3.594 | 0.335 | 28.235 | 1.00 | 12.93 |
| | ATOM | 2304 | CA | LEU | B | 354 | -3.556 | 1.575 | 27.472 | 1.00 | 15.33 |
| | ATOM | 2305 | CB | LEU | B | 354 | -4.616 | 1.534 | 26.360 | 1.00 | 16.44 |
| | ATOM | 2306 | CG | LEU | B | 354 | -4.174 | 0.750 | 25.112 | 1.00 | 17.03 |
| 45 | ATOM | 2307 | CD1 | LEU | B | 354 | -5.373 | 0.509 | 24.189 | 1.00 | 16.70 |
| | ATOM | 2308 | CD2 | LEU | B | 354 | -3.069 | 1.531 | 24.384 | 1.00 | 14.52 |
| | ATOM | 2309 | C | LEU | B | 354 | -3.747 | 2.805 | 28.361 | 1.00 | 12.78 |
| | ATOM | 2310 | O | LEU | B | 354 | -3.123 | 3.850 | 28.141 | 1.00 | 14.28 |
| | ATOM | 2311 | N | VAL | B | 355 | -4.600 | 2.682 | 29.369 | 1.00 | 12.60 |
| 50 | ATOM | 2312 | CA | VAL | B | 355 | -4.844 | 3.791 | 30.279 | 1.00 | 16.78 |
| | ATOM | 2313 | CB | VAL | B | 355 | -5.925 | 3.429 | 31.327 | 1.00 | 16.84 |
| | ATOM | 2314 | CG1 | VAL | B | 355 | -6.070 | 4.561 | 32.344 | 1.00 | 19.88 |
| | ATOM | 2315 | CG2 | VAL | B | 355 | -7.254 | 3.187 | 30.639 | 1.00 | 19.33 |
| | ATOM | 2316 | C | VAL | B | 355 | -3.533 | 4.161 | 30.986 | 1.00 | 19.17 |
| 55 | ATOM | 2317 | O | VAL | B | 355 | -3.158 | 5.328 | 31.049 | 1.00 | 17.30 |
| | ATOM | 2318 | N | HIS | B | 356 | -2.826 | 3.160 | 31.499 | 1.00 | 19.68 |
| | ATOM | 2319 | CA | HIS | B | 356 | -1.559 | 3.418 | 32.177 | 1.00 | 20.64 |
| | ATOM | 2320 | CB | HIS | B | 356 | -1.110 | 2.174 | 32.945 | 1.00 | 21.03 |
| | ATOM | 2321 | CG | HIS | B | 356 | -2.018 | 1.818 | 34.085 | 1.00 | 22.88 |
| 60 | ATOM | 2322 | CD2 | HIS | B | 356 | -3.128 | 1.045 | 34.135 | 1.00 | 21.70 |
| | ATOM | 2323 | ND1 | HIS | B | 356 | -1.838 | 2.312 | 35.358 | 1.00 | 19.24 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 2324 | CE1 | HIS | B | 356 | -2.802 | 1.860 | 36.145 | 1.00 | 18.84 |
| | ATOM | 2325 | NE2 | HIS | B | 356 | -3.598 | 1.088 | 35.426 | 1.00 | 17.92 |
| | ATOM | 2326 | C | HIS | B | 356 | -0.479 | 3.861 | 31.184 | 1.00 | 19.67 |
| | ATOM | 2327 | O | HIS | B | 356 | 0.424 | 4.614 | 31.547 | 1.00 | 19.61 |
| | ATOM | 2328 | N | MET | B | 357 | -0.566 | 3.413 | 29.931 | 1.00 | 14.92 |
| 10 | ATOM | 2329 | CA | MET | B | 357 | 0.428 | 3.830 | 28.939 | 1.00 | 15.13 |
| | ATOM | 2330 | CB | MET | B | 357 | 0.239 | 3.099 | 27.604 | 1.00 | 13.94 |
| | ATOM | 2331 | CG | MET | B | 357 | 1.149 | 3.631 | 26.476 | 1.00 | 14.71 |
| | ATOM | 2332 | SD | MET | B | 357 | 0.747 | 3.014 | 24.826 | 1.00 | 17.75 |
| | ATOM | 2333 | CE | MET | B | 357 | 0.746 | 1.222 | 25.122 | 1.00 | 15.21 |
| 15 | ATOM | 2334 | C | MET | B | 357 | 0.316 | 5.334 | 28.699 | 1.00 | 14.94 |
| | ATOM | 2335 | O | MET | B | 357 | 1.319 | 6.031 | 28.560 | 1.00 | 17.02 |
| | ATOM | 2336 | N | ILE | B | 358 | -0.909 | 5.839 | 28.659 | 1.00 | 18.01 |
| | ATOM | 2337 | CA | ILE | B | 358 | -1.122 | 7.263 | 28.423 | 1.00 | 19.77 |
| | ATOM | 2338 | CB | ILE | B | 358 | -2.634 | 7.577 | 28.287 | 1.00 | 23.11 |
| 20 | ATOM | 2339 | CG2 | ILE | B | 358 | -2.879 | 9.080 | 28.450 | 1.00 | 25.00 |
| | ATOM | 2340 | CG1 | ILE | B | 358 | -3.137 | 7.105 | 26.913 | 1.00 | 24.19 |
| | ATOM | 2341 | CD1 | ILE | B | 358 | -4.600 | 6.653 | 26.890 | 1.00 | 20.17 |
| | ATOM | 2342 | C | ILE | B | 358 | -0.501 | 8.100 | 29.550 | 1.00 | 22.93 |
| | ATOM | 2343 | O | ILE | B | 358 | 0.080 | 9.153 | 29.299 | 1.00 | 23.33 |
| 25 | ATOM | 2344 | N | ASN | B | 359 | -0.619 | 7.631 | 30.790 | 1.00 | 22.34 |
| | ATOM | 2345 | CA | ASN | B | 359 | -0.029 | 8.341 | 31.924 | 1.00 | 23.24 |
| | ATOM | 2346 | CB | ASN | B | 359 | -0.480 | 7.726 | 33.224 | 1.00 | 25.10 |
| | ATOM | 2347 | CG | ASN | B | 359 | -1.831 | 8.171 | 33.649 | 1.00 | 32.65 |
| | ATOM | 2348 | OD1 | ASN | B | 359 | -2.421 | 9.069 | 33.042 | 1.00 | 32.98 |
| 30 | ATOM | 2349 | ND2 | ASN | B | 359 | -2.364 | 7.549 | 34.691 | 1.00 | 33.87 |
| | ATOM | 2350 | C | ASN | B | 359 | 1.473 | 8.306 | 31.837 | 1.00 | 24.77 |
| | ATOM | 2351 | O | ASN | B | 359 | 2.152 | 9.285 | 32.149 | 1.00 | 24.19 |
| | ATOM | 2352 | N | TRP | B | 360 | 1.995 | 7.149 | 31.438 | 1.00 | 20.82 |
| | ATOM | 2353 | CA | TRP | B | 360 | 3.439 | 6.965 | 31.310 | 1.00 | 19.29 |
| 35 | ATOM | 2354 | CB | TRP | B | 360 | 3.754 | 5.524 | 30.878 | 1.00 | 18.59 |
| | ATOM | 2355 | CG | TRP | B | 360 | 5.085 | 5.363 | 30.176 | 1.00 | 18.21 |
| | ATOM | 2356 | CD2 | TRP | B | 360 | 5.310 | 5.308 | 28.756 | 1.00 | 14.38 |
| | ATOM | 2357 | CE2 | TRP | B | 360 | 6.698 | 5.129 | 28.561 | 1.00 | 13.42 |
| | ATOM | 2358 | CE3 | TRP | B | 360 | 4.475 | 5.392 | 27.633 | 1.00 | 15.52 |
| 40 | ATOM | 2359 | CD1 | TRP | B | 360 | 6.306 | 5.221 | 30.762 | 1.00 | 13.34 |
| | ATOM | 2360 | NE1 | TRP | B | 360 | 7.283 | 5.078 | 29.800 | 1.00 | 16.05 |
| | ATOM | 2361 | CZ2 | TRP | B | 360 | 7.272 | 5.032 | 27.288 | 1.00 | 16.84 |
| | ATOM | 2362 | CZ3 | TRP | B | 360 | 5.045 | 5.296 | 26.363 | 1.00 | 15.11 |
| | ATOM | 2363 | CH2 | TRP | B | 360 | 6.431 | 5.115 | 26.202 | 1.00 | 16.12 |
| 45 | ATOM | 2364 | C | TRP | B | 360 | 3.979 | 7.939 | 30.273 | 1.00 | 20.13 |
| | ATOM | 2365 | O | TRP | B | 360 | 4.991 | 8.606 | 30.497 | 1.00 | 17.26 |
| | ATOM | 2366 | N | ALA | B | 361 | 3.295 | 8.012 | 29.135 | 1.00 | 19.34 |
| | ATOM | 2367 | CA | ALA | B | 361 | 3.708 | 8.900 | 28.051 | 1.00 | 22.01 |
| | ATOM | 2368 | CB | ALA | B | 361 | 2.682 | 8.855 | 26.921 | 1.00 | 19.53 |
| 50 | ATOM | 2369 | C | ALA | B | 361 | 3.883 | 10.336 | 28.552 | 1.00 | 22.39 |
| | ATOM | 2370 | O | ALA | B | 361 | 4.858 | 11.005 | 28.210 | 1.00 | 19.57 |
| | ATOM | 2371 | N | LYS | B | 362 | 2.932 | 10.794 | 29.361 | 1.00 | 21.96 |
| | ATOM | 2372 | CA | LYS | B | 362 | 2.966 | 12.139 | 29.923 | 1.00 | 26.45 |
| | ATOM | 2373 | CB | LYS | B | 362 | 1.741 | 12.363 | 30.811 | 1.00 | 29.79 |
| 55 | ATOM | 2374 | CG | LYS | B | 362 | 0.426 | 12.417 | 30.064 | 1.00 | 33.57 |
| | ATOM | 2375 | CD | LYS | B | 362 | -0.563 | 13.304 | 30.805 | 1.00 | 36.83 |
| | ATOM | 2376 | CE | LYS | B | 362 | -1.620 | 12.490 | 31.512 | 1.00 | 36.89 |
| | ATOM | 2377 | NZ | LYS | B | 362 | -2.873 | 13.276 | 31.664 | 1.00 | 39.07 |
| | ATOM | 2378 | C | LYS | B | 362 | 4.223 | 12.379 | 30.757 | 1.00 | 27.77 |
| 60 | ATOM | 2379 | O | LYS | B | 362 | 4.661 | 13.517 | 30.922 | 1.00 | 26.93 |
| | ATOM | 2380 | N | ARG | B | 363 | 4.805 | 11.302 | 31.278 | 1.00 | 26.61 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 2381 | CA | ARG | B | 363 | 5.996 | 11.414 | 32.109 | 1.00 | 27.74 |
| | ATOM | 2382 | CB | ARG | B | 363 | 5.887 | 10.457 | 33.298 | 1.00 | 28.93 |
| | ATOM | 2383 | CG | ARG | B | 363 | 4.650 | 10.704 | 34.158 | 1.00 | 36.07 |
| | ATOM | 2384 | CD | ARG | B | 363 | 4.569 | 9.745 | 35.344 | 1.00 | 42.83 |
| | ATOM | 2385 | NE | ARG | B | 363 | 4.477 | 8.344 | 34.928 | 1.00 | 49.79 |
| 10 | ATOM | 2386 | CZ | ARG | B | 363 | 3.395 | 7.582 | 35.080 | 1.00 | 51.48 |
| | ATOM | 2387 | NH1 | ARG | B | 363 | 2.300 | 8.081 | 35.648 | 1.00 | 52.17 |
| | ATOM | 2388 | NH2 | ARG | B | 363 | 3.405 | 6.316 | 34.668 | 1.00 | 40.24 |
| | ATOM | 2389 | C | ARG | B | 363 | 7.308 | 11.190 | 31.367 | 1.00 | 25.80 |
| | ATOM | 2390 | O | ARG | B | 363 | 8.374 | 11.183 | 31.975 | 1.00 | 29.36 |
| 15 | ATOM | 2391 | N | VAL | B | 364 | 7.231 | 11.009 | 30.053 | 1.00 | 24.28 |
| | ATOM | 2392 | CA | VAL | B | 364 | 8.431 | 10.823 | 29.248 | 1.00 | 21.87 |
| | ATOM | 2393 | CB | VAL | B | 364 | 8.116 | 10.048 | 27.947 | 1.00 | 21.84 |
| | ATOM | 2394 | CG1 | VAL | B | 364 | 9.267 | 10.184 | 26.968 | 1.00 | 15.85 |
| | ATOM | 2395 | CG2 | VAL | B | 364 | 7.860 | 8.560 | 28.268 | 1.00 | 16.24 |
| 20 | ATOM | 2396 | C | VAL | B | 364 | 8.925 | 12.241 | 28.923 | 1.00 | 28.14 |
| | ATOM | 2397 | O | VAL | B | 364 | 8.219 | 13.023 | 28.285 | 1.00 | 24.24 |
| | ATOM | 2398 | N | PRO | B | 365 | 10.141 | 12.591 | 29.375 | 1.00 | 28.57 |
| | ATOM | 2399 | CD | PRO | B | 365 | 11.061 | 11.726 | 30.137 | 1.00 | 30.58 |
| | ATOM | 2400 | CA | PRO | B | 365 | 10.719 | 13.919 | 29.138 | 1.00 | 32.16 |
| 25 | ATOM | 2401 | CB | PRO | B | 365 | 12.189 | 13.739 | 29.507 | 1.00 | 32.70 |
| | ATOM | 2402 | CG | PRO | B | 365 | 12.170 | 12.671 | 30.545 | 1.00 | 33.35 |
| | ATOM | 2403 | C | PRO | B | 365 | 10.546 | 14.464 | 27.726 | 1.00 | 32.22 |
| | ATOM | 2404 | O | PRO | B | 365 | 11.056 | 13.897 | 26.766 | 1.00 | 37.04 |
| | ATOM | 2405 | N | GLY | B | 366 | 9.821 | 15.570 | 27.609 | 1.00 | 34.09 |
| 30 | ATOM | 2406 | CA | GLY | B | 366 | 9.612 | 16.182 | 26.310 | 1.00 | 32.54 |
| | ATOM | 2407 | C | GLY | B | 366 | 8.241 | 15.969 | 25.700 | 1.00 | 33.46 |
| | ATOM | 2408 | O | GLY | B | 366 | 7.791 | 16.779 | 24.886 | 1.00 | 33.73 |
| | ATOM | 2409 | N | PHE | B | 367 | 7.564 | 14.895 | 26.096 | 1.00 | 31.08 |
| | ATOM | 2410 | CA | PHE | B | 367 | 6.250 | 14.593 | 25.542 | 1.00 | 28.60 |
| 35 | ATOM | 2411 | CB | PHE | B | 367 | 5.745 | 13.244 | 26.058 | 1.00 | 25.96 |
| | ATOM | 2412 | CG | PHE | B | 367 | 4.629 | 12.671 | 25.239 | 1.00 | 22.75 |
| | ATOM | 2413 | CD1 | PHE | B | 367 | 3.313 | 12.771 | 25.669 | 1.00 | 22.62 |
| | ATOM | 2414 | CD2 | PHE | B | 367 | 4.897 | 12.025 | 24.033 | 1.00 | 22.29 |
| | ATOM | 2415 | CE1 | PHE | B | 367 | 2.272 | 12.233 | 24.914 | 1.00 | 25.63 |
| 40 | ATOM | 2416 | CE2 | PHE | B | 367 | 3.867 | 11.486 | 23.272 | 1.00 | 20.82 |
| | ATOM | 2417 | CZ | PHE | B | 367 | 2.553 | 11.588 | 23.711 | 1.00 | 25.50 |
| | ATOM | 2418 | C | PHE | B | 367 | 5.178 | 15.646 | 25.781 | 1.00 | 26.79 |
| | ATOM | 2419 | O | PHE | B | 367 | 4.458 | 16.001 | 24.854 | 1.00 | 23.37 |
| | ATOM | 2420 | N | VAL | B | 368 | 5.049 | 16.143 | 27.009 | 1.00 | 31.26 |
| 45 | ATOM | 2421 | CA | VAL | B | 368 | 4.020 | 17.151 | 27.277 | 1.00 | 35.71 |
| | ATOM | 2422 | CB | VAL | B | 368 | 3.817 | 17.412 | 28.795 | 1.00 | 35.98 |
| | ATOM | 2423 | CG1 | VAL | B | 368 | 2.944 | 16.320 | 29.392 | 1.00 | 37.64 |
| | ATOM | 2424 | CG2 | VAL | B | 368 | 5.157 | 17.495 | 29.508 | 1.00 | 35.81 |
| | ATOM | 2425 | C | VAL | B | 368 | 4.328 | 18.482 | 26.598 | 1.00 | 35.87 |
| 50 | ATOM | 2426 | O | VAL | B | 368 | 3.450 | 19.330 | 26.457 | 1.00 | 37.71 |
| | ATOM | 2427 | N | ASP | B | 369 | 5.572 | 18.665 | 26.175 | 1.00 | 35.49 |
| | ATOM | 2428 | CA | ASP | B | 369 | 5.950 | 19.904 | 25.503 | 1.00 | 36.54 |
| | ATOM | 2429 | CB | ASP | B | 369 | 7.466 | 19.963 | 25.309 | 1.00 | 39.79 |
| | ATOM | 2430 | CG | ASP | B | 369 | 8.213 | 20.169 | 26.615 | 1.00 | 44.33 |
| 55 | ATOM | 2431 | OD1 | ASP | B | 369 | 9.409 | 19.807 | 26.684 | 1.00 | 48.45 |
| | ATOM | 2432 | OD2 | ASP | B | 369 | 7.604 | 20.693 | 27.572 | 1.00 | 43.27 |
| | ATOM | 2433 | C | ASP | B | 369 | 5.248 | 19.997 | 24.149 | 1.00 | 34.49 |
| | ATOM | 2434 | O | ASP | B | 369 | 5.131 | 21.074 | 23.571 | 1.00 | 34.51 |
| | ATOM | 2435 | N | LEU | B | 370 | 4.776 | 18.859 | 23.653 | 1.00 | 30.97 |
| 60 | ATOM | 2436 | CA | LEU | B | 370 | 4.086 | 18.809 | 22.370 | 1.00 | 29.80 |
| | ATOM | 2437 | CB | LEU | B | 370 | 4.145 | 17.389 | 21.799 | 1.00 | 27.27 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 2438 | CG | LEU | B | 370 | 5.522 | 16.733 | 21.688 | 1.00 | 28.07 |
| | ATOM | 2439 | CD1 | LEU | B | 370 | 5.353 | 15.242 | 21.400 | 1.00 | 30.38 |
| | ATOM | 2440 | CD2 | LEU | B | 370 | 6.316 | 17.396 | 20.574 | 1.00 | 22.82 |
| | ATOM | 2441 | C | LEU | B | 370 | 2.628 | 19.218 | 22.521 | 1.00 | 28.04 |
| | ATOM | 2442 | O | LEU | B | 370 | 2.066 | 19.151 | 23.611 | 1.00 | 29.71 |
| 10 | ATOM | 2443 | N | THR | B | 371 | 2.011 | 19.645 | 21.425 | 1.00 | 28.70 |
| | ATOM | 2444 | CA | THR | B | 371 | 0.602 | 20.014 | 21.474 | 1.00 | 30.31 |
| | ATOM | 2445 | CB | THR | B | 371 | 0.150 | 20.690 | 20.163 | 1.00 | 31.96 |
| | ATOM | 2446 | OG1 | THR | B | 371 | 0.284 | 19.763 | 19.080 | 1.00 | 29.49 |
| | ATOM | 2447 | CG2 | THR | B | 371 | 0.991 | 21.930 | 19.878 | 1.00 | 29.98 |
| 15 | ATOM | 2448 | C | THR | B | 371 | -0.208 | 18.726 | 21.666 | 1.00 | 30.59 |
| | ATOM | 2449 | O | THR | B | 371 | 0.300 | 17.624 | 21.431 | 1.00 | 27.10 |
| | ATOM | 2450 | N | LEU | B | 372 | -1.461 | 18.863 | 22.087 | 1.00 | 27.65 |
| | ATOM | 2451 | CA | LEU | B | 372 | -2.323 | 17.702 | 22.303 | 1.00 | 30.86 |
| | ATOM | 2452 | CB | LEU | B | 372 | -3.722 | 18.147 | 22.737 | 1.00 | 30.11 |
| 20 | ATOM | 2453 | CG | LEU | B | 372 | -4.715 | 17.006 | 22.960 | 1.00 | 32.80 |
| | ATOM | 2454 | CD1 | LEU | B | 372 | -4.231 | 16.147 | 24.126 | 1.00 | 34.10 |
| | ATOM | 2455 | CD2 | LEU | B | 372 | -6.105 | 17.562 | 23.246 | 1.00 | 31.16 |
| | ATOM | 2456 | C | LEU | B | 372 | -2.437 | 16.863 | 21.034 | 1.00 | 31.77 |
| | ATOM | 2457 | O | LEU | B | 372 | -2.417 | 15.629 | 21.078 | 1.00 | 27.06 |
| 25 | ATOM | 2458 | N | HIS | B | 373 | -2.564 | 17.548 | 19.905 | 1.00 | 31.30 |
| | ATOM | 2459 | CA | HIS | B | 373 | -2.685 | 16.888 | 18.614 | 1.00 | 31.35 |
| | ATOM | 2460 | CB | HIS | B | 373 | -2.844 | 17.935 | 17.503 | 1.00 | 34.30 |
| | ATOM | 2461 | CG | HIS | B | 373 | -2.503 | 17.430 | 16.132 | 1.00 | 41.27 |
| | ATOM | 2462 | CD2 | HIS | B | 373 | -3.293 | 17.105 | 15.079 | 1.00 | 42.50 |
| 30 | ATOM | 2463 | ND1 | HIS | B | 373 | -1.205 | 17.220 | 15.715 | 1.00 | 43.69 |
| | ATOM | 2464 | CE1 | HIS | B | 373 | -1.210 | 16.787 | 14.465 | 1.00 | 48.87 |
| | ATOM | 2465 | NE2 | HIS | B | 373 | -2.465 | 16.708 | 14.056 | 1.00 | 43.72 |
| | ATOM | 2466 | C | HIS | B | 373 | -1.468 | 16.012 | 18.337 | 1.00 | 28.29 |
| | ATOM | 2467 | O | HIS | B | 373 | -1.610 | 14.878 | 17.897 | 1.00 | 30.21 |
| 35 | ATOM | 2468 | N | ASP | B | 374 | -0.275 | 16.541 | 18.589 | 1.00 | 28.85 |
| | ATOM | 2469 | CA | ASP | B | 374 | 0.950 | 15.783 | 18.350 | 1.00 | 28.28 |
| | ATOM | 2470 | CB | ASP | B | 374 | 2.178 | 16.678 | 18.535 | 1.00 | 31.33 |
| | ATOM | 2471 | CG | ASP | B | 374 | 2.433 | 17.577 | 17.333 | 1.00 | 39.07 |
| | ATOM | 2472 | OD1 | ASP | B | 374 | 3.195 | 18.557 | 17.478 | 1.00 | 40.60 |
| 40 | ATOM | 2473 | OD2 | ASP | B | 374 | 1.874 | 17.305 | 16.246 | 1.00 | 38.64 |
| | ATOM | 2474 | C | ASP | B | 374 | 1.029 | 14.592 | 19.303 | 1.00 | 29.05 |
| | ATOM | 2475 | O | ASP | B | 374 | 1.432 | 13.494 | 18.908 | 1.00 | 24.26 |
| | ATOM | 2476 | N | GLN | B | 375 | 0.642 | 14.814 | 20.556 | 1.00 | 24.52 |
| | ATOM | 2477 | CA | GLN | B | 375 | 0.667 | 13.749 | 21.547 | 1.00 | 27.37 |
| 45 | ATOM | 2478 | CB | GLN | B | 375 | 0.213 | 14.270 | 22.901 | 1.00 | 26.66 |
| | ATOM | 2479 | CG | GLN | B | 375 | 1.164 | 15.236 | 23.563 | 1.00 | 29.74 |
| | ATOM | 2480 | CD | GLN | B | 375 | 0.623 | 15.691 | 24.890 | 1.00 | 33.13 |
| | ATOM | 2481 | OE1 | GLN | B | 375 | -0.044 | 14.953 | 25.602 | 1.00 | 32.82 |
| | ATOM | 2482 | NE2 | GLN | B | 375 | 0.895 | 16.953 | 25.236 | 1.00 | 33.98 |
| 50 | ATOM | 2483 | C | GLN | B | 375 | -0.259 | 12.630 | 21.104 | 1.00 | 24.52 |
| | ATOM | 2484 | O | GLN | B | 375 | 0.074 | 11.451 | 21.221 | 1.00 | 23.56 |
| | ATOM | 2485 | N | VAL | B | 376 | -1.426 | 13.013 | 20.599 | 1.00 | 21.87 |
| | ATOM | 2486 | CA | VAL | B | 376 | -2.409 | 12.055 | 20.140 | 1.00 | 23.44 |
| | ATOM | 2487 | CB | VAL | B | 376 | -3.718 | 12.760 | 19.717 | 1.00 | 22.09 |
| 55 | ATOM | 2488 | CG1 | VAL | B | 376 | -4.572 | 11.823 | 18.877 | 1.00 | 24.14 |
| | ATOM | 2489 | CG2 | VAL | B | 376 | -4.486 | 13.192 | 20.954 | 1.00 | 16.96 |
| | ATOM | 2490 | C | VAL | B | 376 | -1.852 | 11.257 | 18.965 | 1.00 | 24.15 |
| | ATOM | 2491 | O | VAL | B | 376 | -1.949 | 10.032 | 18.938 | 1.00 | 22.26 |
| | ATOM | 2492 | N | HIS | B | 377 | -1.251 | 11.953 | 18.007 | 1.00 | 25.85 |
| 60 | ATOM | 2493 | CA | HIS | B | 377 | -0.689 | 11.284 | 16.843 | 1.00 | 25.68 |
| | ATOM | 2494 | CB | HIS | B | 377 | -0.078 | 12.306 | 15.886 | 1.00 | 25.27 |

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|----|------|------|-----|------|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 2495 | CG | HIS | B | 377 | 0.535 | 11.690 | 14.667 | 1.00 | 30.63 |
| | ATOM | 2496 | CD2 | HIS | B | 377 | 1.828 | 11.559 | 14.287 | 1.00 | 31.03 |
| | ATOM | 2497 | ND1 | HIS | B | 377 | -0.217 | 11.086 | 13.683 | 1.00 | 35.05 |
| | ATOM | 2498 | CE1 | HIS | B | 377 | 0.588 | 10.607 | 12.750 | 1.00 | 33.12 |
| | ATOM | 2499 | NE2 | HIS | B | 377 | 1.833 | 10.882 | 13.093 | 1.00 | 31.06 |
| 10 | ATOM | 2500 | C | HIS | B | 377 | 0.365 | 10.237 | 17.210 | 1.00 | 24.37 |
| | ATOM | 2501 | O | HIS | B | 377 | 0.321 | 9.109 | 16.719 | 1.00 | 21.47 |
| | ATOM | 2502 | N | LEU | B | 378 | 1.307 | 10.609 | 18.072 | 1.00 | 19.24 |
| | ATOM | 2503 | CA | LEU | B | 378 | 2.365 | 9.691 | 18.474 | 1.00 | 20.09 |
| | ATOM | 2504 | CB | LEU | B | 378 | 3.363 | 10.402 | 19.388 | 1.00 | 18.64 |
| 15 | ATOM | 2505 | CG | LEU | B | 378 | 4.230 | 11.489 | 18.736 | 1.00 | 22.15 |
| | ATOM | 2506 | CD1 | LEU | B | 378 | 5.104 | 12.148 | 19.796 | 1.00 | 22.51 |
| | ATOM | 2507 | CD2 | LEU | B | 378 | 5.094 | 10.885 | 17.638 | 1.00 | 20.68 |
| | ATOM | 2508 | C | LEU | B | 378 | 1.832 | 8.433 | 19.161 | 1.00 | 18.91 |
| | ATOM | 2509 | O | LEU | B | 378 | 2.262 | 7.320 | 18.859 | 1.00 | 17.52 |
| 20 | ATOM | 2510 | N | LEU | B | 379 | 0.888 | 8.610 | 20.077 | 1.00 | 18.25 |
| | ATOM | 2511 | CA | LEU | B | 379 | 0.317 | 7.486 | 20.795 | 1.00 | 18.60 |
| | ATOM | 2512 | CB | LEU | B | 379 | -0.526 | 7.989 | 21.968 | 1.00 | 16.77 |
| | ATOM | 2513 | CG | LEU | B | 379 | 0.292 | 8.353 | 23.214 | 1.00 | 17.90 |
| | ATOM | 2514 | CD1 | LEU | B | 379 | -0.578 | 9.092 | 24.211 | 1.00 | 15.84 |
| 25 | ATOM | 2515 | CD2 | LEU | B | 379 | 0.851 | 7.075 | 23.842 | 1.00 | 22.09 |
| | ATOM | 2516 | C | LEU | B | 379 | -0.518 | 6.605 | 19.872 | 1.00 | 20.17 |
| | ATOM | 2517 | O | LEU | B | 379 | -0.476 | 5.377 | 19.968 | 1.00 | 18.11 |
| | ATOM | 2518 | N | GLU | B | 380 | -1.273 | 7.222 | 18.971 | 1.00 | 19.40 |
| | ATOM | 2519 | CA | GLU | B | 380 | -2.086 | 6.435 | 18.049 | 1.00 | 20.19 |
| 30 | ATOM | 2520 | CB | GLU | B | 380 | -2.994 | 7.350 | 17.222 | 1.00 | 22.43 |
| | ATOM | 2521 | CG | GLU | B | 380 | -4.182 | 7.874 | 18.007 | 1.00 | 25.30 |
| | ATOM | 2522 | CD | GLU | B | 380 | -5.070 | 8.789 | 17.188 | 1.00 | 29.44 |
| | ATOM | 2523 | OE1 | GLU | B | 380 | -6.206 | 9.066 | 17.625 | 1.00 | 31.70 |
| | ATOM | 2524 | OE2 | GLU | B | 380 | -4.631 | 9.230 | 16.110 | 1.00 | 31.75 |
| 35 | ATOM | 2525 | C | GLU | B | 380 | -1.210 | 5.594 | 17.117 | 1.00 | 18.92 |
| | ATOM | 2526 | O | GLU | B | 380 | -1.586 | 4.491 | 16.722 | 1.00 | 19.83 |
| | ATOM | 2527 | N | ACYS | B | 381 | -0.039 | 6.113 | 16.772 | 0.75 | 17.41 |
| | ATOM | 2528 | N | BCYS | B | 381 | -0.035 | 6.113 | 16.779 | 0.25 | 17.76 |
| | ATOM | 2529 | CA | ACYS | B | 381 | 0.860 | 5.384 | 15.887 | 0.75 | 20.19 |
| 40 | ATOM | 2530 | CA | BCYS | B | 381 | 0.875 | 5.407 | 15.884 | 0.25 | 17.50 |
| | ATOM | 2531 | CB | ACYS | B | 381 | 1.870 | 6.342 | 15.248 | 0.75 | 24.20 |
| | ATOM | 2532 | CB | BCYS | B | 381 | 1.830 | 6.406 | 15.226 | 0.25 | 16.63 |
| | ATOM | 2533 | SG | ACYS | B | 381 | 1.167 | 7.518 | 14.060 | 0.75 | 33.54 |
| | ATOM | 2534 | SG | BCYS | B | 381 | 3.048 | 5.656 | 14.128 | 0.25 | 10.36 |
| 45 | ATOM | 2535 | C | ACYS | B | 381 | 1.626 | 4.269 | 16.592 | 0.75 | 20.59 |
| | ATOM | 2536 | C | BCYS | B | 381 | 1.689 | 4.305 | 16.561 | 0.25 | 19.19 |
| | ATOM | 2537 | O | ACYS | B | 381 | 1.737 | 3.161 | 16.069 | 0.75 | 19.16 |
| | ATOM | 2538 | O | BCYS | B | 381 | 1.904 | 3.241 | 15.982 | 0.25 | 19.25 |
| | ATOM | 2539 | N | ALA | B | 382 | 2.134 | 4.560 | 17.785 | 1.00 | 19.04 |
| 50 | ATOM | 2540 | CA | ALA | B | 382 | 2.955 | 3.602 | 18.530 | 1.00 | 20.27 |
| | ATOM | 2541 | CB | ALA | B | 382 | 4.135 | 4.364 | 19.143 | 1.00 | 18.68 |
| | ATOM | 2542 | C | ALA | B | 382 | 2.356 | 2.702 | 19.607 | 1.00 | 16.82 |
| | ATOM | 2543 | O | ALA | B | 382 | 3.070 | 1.852 | 20.142 | 1.00 | 13.37 |
| | ATOM | 2544 | N | TRP | B | 383 | 1.074 | 2.855 | 19.916 | 1.00 | 15.30 |
| 55 | ATOM | 2545 | CA | TRP | B | 383 | 0.487 | 2.089 | 21.013 | 1.00 | 15.80 |
| | ATOM | 2546 | CB | TRP | B | 383 | -1.009 | 2.410 | 21.160 | 1.00 | 16.63 |
| | ATOM | 2547 | CG | TRP | B | 383 | -1.871 | 1.775 | 20.129 | 1.00 | 19.93 |
| | ATOM | 2548 | CD2 | TRP | B | 383 | -2.493 | 0.483 | 20.198 | 1.00 | 20.80 |
| | ATOM | 2549 | CE2 | TRP | B | 383 | -3.226 | 0.309 | 19.003 | 1.00 | 19.27 |
| 60 | ATOM | 2550 | CE3 | TRP | B | 383 | -2.506 | -0.542 | 21.155 | 1.00 | 21.32 |
| | ATOM | 2551 | CD1 | TRP | B | 383 | -2.236 | 2.312 | 18.933 | 1.00 | 18.59 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 2552 | NE1 | TRP | B | 383 | -3.051 | 1.439 | 18.250 | 1.00 | 23.67 |
| | ATOM | 2553 | CZ2 | TRP | B | 383 | -3.963 | -0.853 | 18.733 | 1.00 | 21.55 |
| | ATOM | 2554 | CZ3 | TRP | B | 383 | -3.243 | -1.702 | 20.888 | 1.00 | 20.29 |
| | ATOM | 2555 | CH2 | TRP | B | 383 | -3.960 | -1.844 | 19.686 | 1.00 | 19.03 |
| | ATOM | 2556 | C | TRP | B | 383 | 0.701 | 0.579 | 21.020 | 1.00 | 17.35 |
| 10 | ATOM | 2557 | O | TRP | B | 383 | 0.982 | 0.010 | 22.077 | 1.00 | 13.92 |
| | ATOM | 2558 | N | LEU | B | 384 | 0.568 | -0.087 | 19.879 | 1.00 | 14.07 |
| | ATOM | 2559 | CA | LEU | B | 384 | 0.773 | -1.532 | 19.903 | 1.00 | 15.98 |
| | ATOM | 2560 | CB | LEU | B | 384 | 0.181 | -2.200 | 18.656 | 1.00 | 12.19 |
| | ATOM | 2561 | CG | LEU | B | 384 | 0.173 | -3.735 | 18.720 | 1.00 | 12.97 |
| 15 | ATOM | 2562 | CD1 | LEU | B | 384 | -0.352 | -4.240 | 20.089 | 1.00 | 10.65 |
| | ATOM | 2563 | CD2 | LEU | B | 384 | -0.707 | -4.259 | 17.586 | 1.00 | 17.84 |
| | ATOM | 2564 | C | LEU | B | 384 | 2.262 | -1.861 | 20.034 | 1.00 | 14.64 |
| | ATOM | 2565 | O | LEU | B | 384 | 2.627 | -2.833 | 20.690 | 1.00 | 13.78 |
| | ATOM | 2566 | N | GLU | B | 385 | 3.116 | -1.046 | 19.414 | 1.00 | 14.96 |
| 20 | ATOM | 2567 | CA | GLU | B | 385 | 4.565 | -1.260 | 19.509 | 1.00 | 13.79 |
| | ATOM | 2568 | CB | GLU | B | 385 | 5.336 | -0.179 | 18.739 | 1.00 | 15.34 |
| | ATOM | 2569 | CG | GLU | B | 385 | 5.297 | -0.312 | 17.207 | 1.00 | 15.38 |
| | ATOM | 2570 | CD | GLU | B | 385 | 6.162 | 0.738 | 16.520 | 1.00 | 23.97 |
| | ATOM | 2571 | OE1 | GLU | B | 385 | 7.381 | 0.500 | 16.358 | 1.00 | 21.03 |
| 25 | ATOM | 2572 | OE2 | GLU | B | 385 | 5.622 | 1.808 | 16.149 | 1.00 | 22.19 |
| | ATOM | 2573 | C | GLU | B | 385 | 4.963 | -1.161 | 20.987 | 1.00 | 15.79 |
| | ATOM | 2574 | O | GLU | B | 385 | 5.788 | -1.942 | 21.463 | 1.00 | 15.04 |
| | ATOM | 2575 | N | ILE | B | 386 | 4.389 | -0.213 | 21.690 | 1.00 | 13.32 |
| | ATOM | 2576 | CA | ILE | B | 386 | 4.723 | -0.019 | 23.108 | 1.00 | 14.06 |
| 30 | ATOM | 2577 | CB | ILE | B | 386 | 4.173 | 1.326 | 23.614 | 1.00 | 15.36 |
| | ATOM | 2578 | CG2 | ILE | B | 386 | 4.374 | 1.451 | 25.130 | 1.00 | 15.97 |
| | ATOM | 2579 | CG1 | ILE | B | 386 | 4.910 | 2.476 | 22.907 | 1.00 | 17.95 |
| | ATOM | 2580 | CD1 | ILE | B | 386 | 4.118 | 3.768 | 22.874 | 1.00 | 21.12 |
| | ATOM | 2581 | C | ILE | B | 386 | 4.227 | -1.164 | 23.993 | 1.00 | 14.97 |
| 35 | ATOM | 2582 | O | ILE | B | 386 | 4.905 | -1.560 | 24.941 | 1.00 | 19.60 |
| | ATOM | 2583 | N | LEU | B | 387 | 3.038 | -1.675 | 23.709 | 1.00 | 15.18 |
| | ATOM | 2584 | CA | LEU | B | 387 | 2.516 | -2.791 | 24.478 | 1.00 | 15.98 |
| | ATOM | 2585 | CB | LEU | B | 387 | 1.070 | -3.097 | 24.080 | 1.00 | 17.15 |
| | ATOM | 2586 | CG | LEU | B | 387 | -0.031 | -2.113 | 24.486 | 1.00 | 19.65 |
| 40 | ATOM | 2587 | CD1 | LEU | B | 387 | -1.371 | -2.628 | 23.972 | 1.00 | 17.77 |
| | ATOM | 2588 | CD2 | LEU | B | 387 | -0.075 | -1.966 | 26.002 | 1.00 | 15.38 |
| | ATOM | 2589 | C | LEU | B | 387 | 3.391 | -4.013 | 24.180 | 1.00 | 14.69 |
| | ATOM | 2590 | O | LEU | B | 387 | 3.712 | -4.792 | 25.076 | 1.00 | 14.03 |
| | ATOM | 2591 | N | MET | B | 388 | 3.785 | -4.178 | 22.921 | 1.00 | 16.43 |
| 45 | ATOM | 2592 | CA | MET | B | 388 | 4.602 | -5.329 | 22.547 | 1.00 | 16.67 |
| | ATOM | 2593 | CB | MET | B | 388 | 4.673 | -5.460 | 21.026 | 1.00 | 14.83 |
| | ATOM | 2594 | CG | MET | B | 388 | 3.403 | -6.066 | 20.453 | 1.00 | 13.91 |
| | ATOM | 2595 | SD | MET | B | 388 | 3.364 | -6.193 | 18.675 | 1.00 | 17.23 |
| | ATOM | 2596 | CE | MET | B | 388 | 1.906 | -7.225 | 18.511 | 1.00 | 14.97 |
| 50 | ATOM | 2597 | C | MET | B | 388 | 6.004 | -5.332 | 23.133 | 1.00 | 20.19 |
| | ATOM | 2598 | O | MET | B | 388 | 6.460 | -6.366 | 23.636 | 1.00 | 21.50 |
| | ATOM | 2599 | N | ILE | B | 389 | 6.707 | -4.203 | 23.074 | 1.00 | 15.34 |
| | ATOM | 2600 | CA | ILE | B | 389 | 8.044 | -4.209 | 23.634 | 1.00 | 15.59 |
| | ATOM | 2601 | CB | ILE | B | 389 | 8.836 | -2.911 | 23.322 | 1.00 | 14.95 |
| 55 | ATOM | 2602 | CG2 | ILE | B | 389 | 8.330 | -1.746 | 24.158 | 1.00 | 12.81 |
| | ATOM | 2603 | CG1 | ILE | B | 389 | 10.325 | -3.164 | 23.602 | 1.00 | 17.24 |
| | ATOM | 2604 | CD1 | ILE | B | 389 | 11.228 | -1.972 | 23.357 | 1.00 | 15.65 |
| | ATOM | 2605 | C | ILE | B | 389 | 7.950 | -4.446 | 25.147 | 1.00 | 14.30 |
| | ATOM | 2606 | O | ILE | B | 389 | 8.844 | -5.044 | 25.739 | 1.00 | 18.72 |
| 60 | ATOM | 2607 | N | GLY | B | 390 | 6.855 | -4.007 | 25.761 | 1.00 | 13.99 |
| | ATOM | 2608 | CA | GLY | B | 390 | 6.681 | -4.219 | 27.189 | 1.00 | 14.87 |

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 2609 | C | GLY | B | 390 | 6.444 | -5.702 | 27.463 | 1.00 | 18.54 |
| | ATOM | 2610 | O | GLY | B | 390 | 6.989 | -6.282 | 28.403 | 1.00 | 16.54 |
| | ATOM | 2611 | N | LEU | B | 391 | 5.623 | -6.325 | 26.628 | 1.00 | 16.15 |
| | ATOM | 2612 | CA | LEU | B | 391 | 5.334 | -7.743 | 26.775 | 1.00 | 18.91 |
| | ATOM | 2613 | CB | LEU | B | 391 | 4.332 | -8.179 | 25.699 | 1.00 | 19.55 |
| 10 | ATOM | 2614 | CG | LEU | B | 391 | 4.157 | -9.689 | 25.457 | 1.00 | 20.91 |
| | ATOM | 2615 | CD1 | LEU | B | 391 | 3.580 | -10.351 | 26.699 | 1.00 | 19.41 |
| | ATOM | 2616 | CD2 | LEU | B | 391 | 3.232 | -9.913 | 24.268 | 1.00 | 20.70 |
| | ATOM | 2617 | C | LEU | B | 391 | 6.649 | -8.518 | 26.625 | 1.00 | 20.31 |
| | ATOM | 2618 | O | LEU | B | 391 | 7.002 | -9.352 | 27.465 | 1.00 | 18.66 |
| 15 | ATOM | 2619 | N | VAL | B | 392 | 7.378 | -8.215 | 25.557 | 1.00 | 18.71 |
| | ATOM | 2620 | CA | VAL | B | 392 | 8.649 | -8.868 | 25.278 | 1.00 | 19.51 |
| | ATOM | 2621 | CB | VAL | B | 392 | 9.288 | -8.281 | 24.005 | 1.00 | 23.77 |
| | ATOM | 2622 | CG1 | VAL | B | 392 | 10.751 | -8.687 | 23.920 | 1.00 | 24.63 |
| | ATOM | 2623 | CG2 | VAL | B | 392 | 8.520 | -8.773 | 22.767 | 1.00 | 19.94 |
| 20 | ATOM | 2624 | C | VAL | B | 392 | 9.615 | -8.707 | 26.450 | 1.00 | 22.80 |
| | ATOM | 2625 | O | VAL | B | 392 | 10.336 | -9.637 | 26.811 | 1.00 | 19.36 |
| | ATOM | 2626 | N | TRP | B | 393 | 9.617 | -7.522 | 27.046 | 1.00 | 22.10 |
| | ATOM | 2627 | CA | TRP | B | 393 | 10.492 | -7.241 | 28.171 | 1.00 | 23.20 |
| | ATOM | 2628 | CB | TRP | B | 393 | 10.388 | -5.773 | 28.578 | 1.00 | 19.22 |
| 25 | ATOM | 2629 | CG | TRP | B | 393 | 11.056 | -5.479 | 29.895 | 1.00 | 22.53 |
| | ATOM | 2630 | CD2 | TRP | B | 393 | 12.453 | -5.591 | 30.193 | 1.00 | 20.36 |
| | ATOM | 2631 | CE2 | TRP | B | 393 | 12.624 | -5.208 | 31.545 | 1.00 | 25.65 |
| | ATOM | 2632 | CE3 | TRP | B | 393 | 13.578 | -5.976 | 29.449 | 1.00 | 22.12 |
| | ATOM | 2633 | CD1 | TRP | B | 393 | 10.452 | -5.046 | 31.044 | 1.00 | 23.02 |
| 30 | ATOM | 2634 | NE1 | TRP | B | 393 | 11.387 | -4.881 | 32.037 | 1.00 | 24.91 |
| | ATOM | 2635 | CZ2 | TRP | B | 393 | 13.876 | -5.200 | 32.171 | 1.00 | 23.00 |
| | ATOM | 2636 | CZ3 | TRP | B | 393 | 14.829 | -5.968 | 30.072 | 1.00 | 23.98 |
| | ATOM | 2637 | CH2 | TRP | B | 393 | 14.964 | -5.582 | 31.423 | 1.00 | 23.20 |
| | ATOM | 2638 | C | TRP | B | 393 | 10.208 | -8.114 | 29.388 | 1.00 | 24.36 |
| 35 | ATOM | 2639 | O | TRP | B | 393 | 11.128 | -8.717 | 29.944 | 1.00 | 23.04 |
| | ATOM | 2640 | N | ARG | B | 394 | 8.952 | -8.189 | 29.819 | 1.00 | 21.29 |
| | ATOM | 2641 | CA | ARG | B | 394 | 8.680 | -9.003 | 30.990 | 1.00 | 22.43 |
| | ATOM | 2642 | CB | ARG | B | 394 | 7.365 | -8.601 | 31.667 | 1.00 | 23.97 |
| | ATOM | 2643 | CG | ARG | B | 394 | 6.259 | -8.149 | 30.759 | 1.00 | 26.16 |
| 40 | ATOM | 2644 | CD | ARG | B | 394 | 5.026 | -7.727 | 31.574 | 1.00 | 20.86 |
| | ATOM | 2645 | NE | ARG | B | 394 | 3.817 | -7.937 | 30.786 | 1.00 | 19.54 |
| | ATOM | 2646 | CZ | ARG | B | 394 | 3.327 | -7.059 | 29.915 | 1.00 | 20.58 |
| | ATOM | 2647 | NH1 | ARG | B | 394 | 3.944 | -5.902 | 29.722 | 1.00 | 17.41 |
| | ATOM | 2648 | NH2 | ARG | B | 394 | 2.229 | -7.347 | 29.220 | 1.00 | 16.82 |
| 45 | ATOM | 2649 | C | ARG | B | 394 | 8.695 | -10.502 | 30.713 | 1.00 | 21.78 |
| | ATOM | 2650 | O | ARG | B | 394 | 8.657 | -11.294 | 31.648 | 1.00 | 23.44 |
| | ATOM | 2651 | N | SER | B | 395 | 8.767 | -10.880 | 29.438 | 1.00 | 17.10 |
| | ATOM | 2652 | CA | SER | B | 395 | 8.805 | -12.289 | 29.041 | 1.00 | 25.08 |
| | ATOM | 2653 | CB | SER | B | 395 | 8.206 | -12.473 | 27.638 | 1.00 | 19.47 |
| 50 | ATOM | 2654 | OG | SER | B | 395 | 6.832 | -12.136 | 27.619 | 1.00 | 21.73 |
| | ATOM | 2655 | C | SER | B | 395 | 10.239 | -12.831 | 29.031 | 1.00 | 26.29 |
| | ATOM | 2656 | O | SER | B | 395 | 10.458 | -14.030 | 28.854 | 1.00 | 23.75 |
| | ATOM | 2657 | N | MET | B | 396 | 11.206 | -11.938 | 29.210 | 1.00 | 30.79 |
| | ATOM | 2658 | CA | MET | B | 396 | 12.620 | -12.307 | 29.205 | 1.00 | 35.07 |
| 55 | ATOM | 2659 | CB | MET | B | 396 | 13.479 | -11.063 | 29.423 | 1.00 | 33.84 |
| | ATOM | 2660 | CG | MET | B | 396 | 14.155 | -10.569 | 28.171 | 1.00 | 36.88 |
| | ATOM | 2661 | SD | MET | B | 396 | 15.149 | -9.127 | 28.491 | 1.00 | 40.96 |
| | ATOM | 2662 | CE | MET | B | 396 | 16.675 | -9.849 | 28.998 | 1.00 | 39.67 |
| | ATOM | 2663 | C | MET | B | 396 | 12.983 | -13.353 | 30.250 | 1.00 | 35.88 |
| 60 | ATOM | 2664 | O | MET | B | 396 | 13.828 | -14.215 | 30.011 | 1.00 | 34.52 |
| | ATOM | 2665 | N | GLU | B | 397 | 12.348 | -13.266 | 31.410 | 1.00 | 36.19 |

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 2666 | CA | GLU | B | 397 | 12.604 | -14.206 | 32.492 | 1.00 | 39.24 |
| | ATOM | 2667 | CB | GLU | B | 397 | 12.153 | -13.605 | 33.821 | 1.00 | 44.38 |
| | ATOM | 2668 | CG | GLU | B | 397 | 12.983 | -12.422 | 34.271 | 1.00 | 54.05 |
| | ATOM | 2669 | CD | GLU | B | 397 | 13.483 | -12.587 | 35.686 | 1.00 | 56.78 |
| | ATOM | 2670 | OE1 | GLU | B | 397 | 13.380 | -11.621 | 36.470 | 1.00 | 60.90 |
| 10 | ATOM | 2671 | OE2 | GLU | B | 397 | 13.975 | -13.688 | 36.013 | 1.00 | 60.82 |
| | ATOM | 2672 | C | GLU | B | 397 | 11.878 | -15.528 | 32.273 | 1.00 | 36.65 |
| | ATOM | 2673 | O | GLU | B | 397 | 12.021 | -16.459 | 33.061 | 1.00 | 35.84 |
| | ATOM | 2674 | N | HIS | B | 398 | 11.100 | -15.609 | 31.202 | 1.00 | 32.14 |
| | ATOM | 2675 | CA | HIS | B | 398 | 10.347 | -16.823 | 30.914 | 1.00 | 29.48 |
| 15 | ATOM | 2676 | CB | HIS | B | 398 | 8.863 | -16.567 | 31.178 | 1.00 | 29.87 |
| | ATOM | 2677 | CG | HIS | B | 398 | 8.582 | -16.111 | 32.574 | 1.00 | 31.80 |
| | ATOM | 2678 | CD2 | HIS | B | 398 | 8.215 | -16.801 | 33.678 | 1.00 | 29.12 |
| | ATOM | 2679 | ND1 | HIS | B | 398 | 8.727 | -14.799 | 32.972 | 1.00 | 33.27 |
| | ATOM | 2680 | CE1 | HIS | B | 398 | 8.462 | -14.701 | 34.262 | 1.00 | 32.19 |
| 20 | ATOM | 2681 | NE2 | HIS | B | 398 | 8.148 | -15.902 | 34.714 | 1.00 | 33.48 |
| | ATOM | 2682 | C | HIS | B | 398 | 10.556 | -17.317 | 29.492 | 1.00 | 25.95 |
| | ATOM | 2683 | O | HIS | B | 398 | 9.637 | -17.291 | 28.672 | 1.00 | 27.47 |
| | ATOM | 2684 | N | PRO | B | 399 | 11.771 | -17.801 | 29.186 | 1.00 | 29.09 |
| | ATOM | 2685 | CD | PRO | B | 399 | 12.926 | -17.922 | 30.096 | 1.00 | 29.93 |
| 25 | ATOM | 2686 | CA | PRO | B | 399 | 12.079 | -18.300 | 27.845 | 1.00 | 27.40 |
| | ATOM | 2687 | CB | PRO | B | 399 | 13.434 | -18.988 | 28.016 | 1.00 | 32.09 |
| | ATOM | 2688 | CG | PRO | B | 399 | 14.062 | -18.284 | 29.170 | 1.00 | 30.81 |
| | ATOM | 2689 | C | PRO | B | 399 | 11.009 | -19.246 | 27.319 | 1.00 | 29.76 |
| | ATOM | 2690 | O | PRO | B | 399 | 10.552 | -20.137 | 28.035 | 1.00 | 29.18 |
| 30 | ATOM | 2691 | N | GLY | B | 400 | 10.601 | -19.035 | 26.071 | 1.00 | 27.45 |
| | ATOM | 2692 | CA | GLY | B | 400 | 9.588 | -19.884 | 25.466 | 1.00 | 26.93 |
| | ATOM | 2693 | C | GLY | B | 400 | 8.161 | -19.537 | 25.849 | 1.00 | 26.73 |
| | ATOM | 2694 | O | GLY | B | 400 | 7.220 | -20.153 | 25.356 | 1.00 | 28.36 |
| | ATOM | 2695 | N | LYS | B | 401 | 7.996 | -18.554 | 26.727 | 1.00 | 25.50 |
| 35 | ATOM | 2696 | CA | LYS | B | 401 | 6.668 | -18.139 | 27.165 | 1.00 | 23.45 |
| | ATOM | 2697 | CB | LYS | B | 401 | 6.435 | -18.563 | 28.619 | 1.00 | 28.50 |
| | ATOM | 2698 | CG | LYS | B | 401 | 6.476 | -20.069 | 28.879 | 1.00 | 28.58 |
| | ATOM | 2699 | CD | LYS | B | 401 | 6.181 | -20.353 | 30.349 | 1.00 | 35.47 |
| | ATOM | 2700 | CE | LYS | B | 401 | 6.073 | -21.847 | 30.635 | 1.00 | 38.59 |
| 40 | ATOM | 2701 | NZ | LYS | B | 401 | 7.177 | -22.611 | 29.989 | 1.00 | 42.39 |
| | ATOM | 2702 | C | LYS | B | 401 | 6.493 | -16.622 | 27.060 | 1.00 | 21.78 |
| | ATOM | 2703 | O | LYS | B | 401 | 7.465 | -15.872 | 27.035 | 1.00 | 21.45 |
| | ATOM | 2704 | N | LEU | B | 402 | 5.241 | -16.181 | 26.995 | 1.00 | 23.45 |
| | ATOM | 2705 | CA | LEU | B | 402 | 4.929 | -14.759 | 26.925 | 1.00 | 21.37 |
| 45 | ATOM | 2706 | CB | LEU | B | 402 | 4.088 | -14.449 | 25.689 | 1.00 | 18.47 |
| | ATOM | 2707 | CG | LEU | B | 402 | 4.798 | -14.673 | 24.360 | 1.00 | 16.89 |
| | ATOM | 2708 | CD1 | LEU | B | 402 | 3.821 | -14.395 | 23.211 | 1.00 | 21.23 |
| | ATOM | 2709 | CD2 | LEU | B | 402 | 6.011 | -13.760 | 24.277 | 1.00 | 23.15 |
| | ATOM | 2710 | C | LEU | B | 402 | 4.147 | -14.399 | 28.179 | 1.00 | 19.66 |
| 50 | ATOM | 2711 | O | LEU | B | 402 | 3.024 | -14.880 | 28.381 | 1.00 | 18.05 |
| | ATOM | 2712 | N | LEU | B | 403 | 4.743 | -13.559 | 29.019 | 1.00 | 19.54 |
| | ATOM | 2713 | CA | LEU | B | 403 | 4.099 | -13.148 | 30.259 | 1.00 | 20.21 |
| | ATOM | 2714 | CB | LEU | B | 403 | 5.155 | -12.856 | 31.332 | 1.00 | 23.16 |
| | ATOM | 2715 | CG | LEU | B | 403 | 4.639 | -12.682 | 32.766 | 1.00 | 29.54 |
| 55 | ATOM | 2716 | CD1 | LEU | B | 403 | 5.519 | -13.450 | 33.728 | 1.00 | 32.67 |
| | ATOM | 2717 | CD2 | LEU | B | 403 | 4.626 | -11.213 | 33.138 | 1.00 | 32.38 |
| | ATOM | 2718 | C | LEU | B | 403 | 3.219 | -11.918 | 30.043 | 1.00 | 20.42 |
| | ATOM | 2719 | O | LEU | B | 403 | 3.638 | -10.787 | 30.291 | 1.00 | 19.18 |
| | ATOM | 2720 | N | PHE | B | 404 | 2.003 | -12.145 | 29.565 | 1.00 | 21.44 |
| 60 | ATOM | 2721 | CA | PHE | B | 404 | 1.066 | -11.053 | 29.340 | 1.00 | 21.69 |
| | ATOM | 2722 | CB | PHE | B | 404 | -0.199 | -11.598 | 28.687 | 1.00 | 17.26 |

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 2723 | CG | PHE | B | 404 | -0.026 | -11.897 | 27.227 | 1.00 | 19.75 |
| | ATOM | 2724 | CD1 | PHE | B | 404 | 0.364 | -13.167 | 26.801 | 1.00 | 17.90 |
| | ATOM | 2725 | CD2 | PHE | B | 404 | -0.210 | -10.897 | 26.280 | 1.00 | 17.04 |
| | ATOM | 2726 | CE1 | PHE | B | 404 | 0.572 | -13.434 | 25.447 | 1.00 | 19.88 |
| | ATOM | 2727 | CE2 | PHE | B | 404 | -0.007 | -11.148 | 24.924 | 1.00 | 18.47 |
| 10 | ATOM | 2728 | CZ | PHE | B | 404 | 0.386 | -12.418 | 24.503 | 1.00 | 16.45 |
| | ATOM | 2729 | C | PHE | B | 404 | 0.768 | -10.403 | 30.685 | 1.00 | 21.95 |
| | ATOM | 2730 | O | PHE | B | 404 | 0.656 | -9.177 | 30.804 | 1.00 | 22.99 |
| | ATOM | 2731 | N | ALA | B | 405 | 0.670 | -11.247 | 31.702 | 1.00 | 21.12 |
| | ATOM | 2732 | CA | ALA | B | 405 | 0.424 | -10.814 | 33.066 | 1.00 | 22.43 |
| 15 | ATOM | 2733 | CB | ALA | B | 405 | -1.074 | -10.603 | 33.304 | 1.00 | 24.69 |
| | ATOM | 2734 | C | ALA | B | 405 | 0.959 | -11.926 | 33.962 | 1.00 | 22.40 |
| | ATOM | 2735 | O | ALA | B | 405 | 1.133 | -13.061 | 33.517 | 1.00 | 21.67 |
| | ATOM | 2736 | N | PRO | B | 406 | 1.246 | -11.612 | 35.230 | 1.00 | 25.60 |
| | ATOM | 2737 | CD | PRO | B | 406 | 1.129 | -10.294 | 35.878 | 1.00 | 23.65 |
| 20 | ATOM | 2738 | CA | PRO | B | 406 | 1.765 | -12.632 | 36.148 | 1.00 | 25.91 |
| | ATOM | 2739 | CB | PRO | B | 406 | 1.899 | -11.882 | 37.475 | 1.00 | 27.04 |
| | ATOM | 2740 | CG | PRO | B | 406 | 2.017 | -10.431 | 37.068 | 1.00 | 26.56 |
| | ATOM | 2741 | C | PRO | B | 406 | 0.876 | -13.873 | 36.259 | 1.00 | 25.12 |
| | ATOM | 2742 | O | PRO | B | 406 | 1.368 | -14.967 | 36.538 | 1.00 | 28.92 |
| 25 | ATOM | 2743 | N | ASN | B | 407 | -0.426 | -13.713 | 36.039 | 1.00 | 23.53 |
| | ATOM | 2744 | CA | ASN | B | 407 | -1.345 | -14.852 | 36.109 | 1.00 | 24.09 |
| | ATOM | 2745 | CB | ASN | B | 407 | -2.553 | -14.526 | 36.986 | 1.00 | 24.08 |
| | ATOM | 2746 | CG | ASN | B | 407 | -3.327 | -13.328 | 36.486 | 1.00 | 26.72 |
| | ATOM | 2747 | OD1 | ASN | B | 407 | -2.851 | -12.574 | 35.635 | 1.00 | 22.65 |
| 30 | ATOM | 2748 | ND2 | ASN | B | 407 | -4.528 | -13.140 | 37.019 | 1.00 | 26.46 |
| | ATOM | 2749 | C | ASN | B | 407 | -1.820 | -15.231 | 34.714 | 1.00 | 26.91 |
| | ATOM | 2750 | O | ASN | B | 407 | -2.859 | -15.870 | 34.548 | 1.00 | 28.68 |
| | ATOM | 2751 | N | LEU | B | 408 | -1.059 | -14.816 | 33.708 | 1.00 | 27.28 |
| | ATOM | 2752 | CA | LEU | B | 408 | -1.387 | -15.124 | 32.327 | 1.00 | 27.23 |
| 35 | ATOM | 2753 | CB | LEU | B | 408 | -2.247 | -14.030 | 31.699 | 1.00 | 26.61 |
| | ATOM | 2754 | CG | LEU | B | 408 | -2.815 | -14.464 | 30.341 | 1.00 | 27.51 |
| | ATOM | 2755 | CD1 | LEU | B | 408 | -3.702 | -15.692 | 30.546 | 1.00 | 28.75 |
| | ATOM | 2756 | CD2 | LEU | B | 408 | -3.598 | -13.330 | 29.694 | 1.00 | 25.48 |
| | ATOM | 2757 | C | LEU | B | 408 | -0.113 | -15.316 | 31.514 | 1.00 | 27.56 |
| 40 | ATOM | 2758 | O | LEU | B | 408 | 0.247 | -14.465 | 30.695 | 1.00 | 26.86 |
| | ATOM | 2759 | N | LEU | B | 409 | 0.553 | -16.426 | 31.759 | 1.00 | 27.54 |
| | ATOM | 2760 | CA | LEU | B | 409 | 1.786 | -16.774 | 31.065 | 1.00 | 31.96 |
| | ATOM | 2761 | CB | LEU | B | 409 | 2.786 | -17.355 | 32.058 | 1.00 | 31.88 |
| | ATOM | 2762 | CG | LEU | B | 409 | 4.186 | -17.703 | 31.562 | 1.00 | 37.72 |
| 45 | ATOM | 2763 | CD1 | LEU | B | 409 | 4.773 | -16.551 | 30.770 | 1.00 | 39.57 |
| | ATOM | 2764 | CD2 | LEU | B | 409 | 5.066 | -18.018 | 32.758 | 1.00 | 41.72 |
| | ATOM | 2765 | C | LEU | B | 409 | 1.401 | -17.805 | 30.009 | 1.00 | 31.53 |
| | ATOM | 2766 | O | LEU | B | 409 | 0.921 | -18.892 | 30.340 | 1.00 | 32.67 |
| | ATOM | 2767 | N | LEU | B | 410 | 1.604 | -17.465 | 28.746 | 1.00 | 29.58 |
| 50 | ATOM | 2768 | CA | LEU | B | 410 | 1.228 | -18.361 | 27.660 | 1.00 | 31.55 |
| | ATOM | 2769 | CB | LEU | B | 410 | 0.192 | -17.672 | 26.762 | 1.00 | 29.83 |
| | ATOM | 2770 | CG | LEU | B | 410 | -1.047 | -17.080 | 27.452 | 1.00 | 28.55 |
| | ATOM | 2771 | CD1 | LEU | B | 410 | -1.770 | -16.135 | 26.501 | 1.00 | 26.92 |
| | ATOM | 2772 | CD2 | LEU | B | 410 | -1.979 | -18.200 | 27.891 | 1.00 | 30.49 |
| 55 | ATOM | 2773 | C | LEU | B | 410 | 2.397 | -18.839 | 26.814 | 1.00 | 33.88 |
| | ATOM | 2774 | O | LEU | B | 410 | 3.427 | -18.170 | 26.726 | 1.00 | 36.49 |
| | ATOM | 2775 | N | ASP | B | 411 | 2.238 | -20.013 | 26.206 | 1.00 | 38.80 |
| | ATOM | 2776 | CA | ASP | B | 411 | 3.275 | -20.562 | 25.336 | 1.00 | 38.39 |
| | ATOM | 2777 | CB | ASP | B | 411 | 3.657 | -21.990 | 25.752 | 1.00 | 44.53 |
| 60 | ATOM | 2778 | CG | ASP | B | 411 | 2.476 | -22.943 | 25.749 | 1.00 | 44.90 |
| | ATOM | 2779 | OD1 | ASP | B | 411 | 1.773 | -23.035 | 24.719 | 1.00 | 45.70 |

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 2780 | OD2 | ASP | B | 411 | 2.254 | -23.603 | 26.786 | 1.00 | 50.54 |
| | ATOM | 2781 | C | ASP | B | 411 | 2.745 | -20.551 | 23.909 | 1.00 | 38.57 |
| | ATOM | 2782 | O | ASP | B | 411 | 1.549 | -20.341 | 23.686 | 1.00 | 36.48 |
| 10 | ATOM | 2783 | N | ARG | B | 412 | 3.635 | -20.777 | 22.949 | 1.00 | 36.85 |
| | ATOM | 2784 | CA | ARG | B | 412 | 3.259 | -20.763 | 21.541 | 1.00 | 38.32 |
| | ATOM | 2785 | CB | ARG | B | 412 | 4.488 | -21.083 | 20.675 | 1.00 | 38.69 |
| | ATOM | 2786 | CG | ARG | B | 412 | 4.361 | -22.314 | 19.799 | 1.00 | 40.05 |
| | ATOM | 2787 | CD | ARG | B | 412 | 5.644 | -22.552 | 19.012 | 1.00 | 42.98 |
| 15 | ATOM | 2788 | NE | ARG | B | 412 | 5.540 | -22.099 | 17.626 | 1.00 | 40.95 |
| | ATOM | 2789 | CZ | ARG | B | 412 | 4.649 | -22.559 | 16.753 | 1.00 | 41.11 |
| | ATOM | 2790 | NH1 | ARG | B | 412 | 3.777 | -23.490 | 17.115 | 1.00 | 44.01 |
| | ATOM | 2791 | NH2 | ARG | B | 412 | 4.632 | -22.091 | 15.515 | 1.00 | 41.28 |
| | ATOM | 2792 | C | ARG | B | 412 | 2.107 | -21.712 | 21.217 | 1.00 | 37.64 |
| 20 | ATOM | 2793 | O | ARG | B | 412 | 1.287 | -21.427 | 20.343 | 1.00 | 36.51 |
| | ATOM | 2794 | N | ASN | B | 413 | 2.041 | -22.834 | 21.923 | 1.00 | 35.32 |
| | ATOM | 2795 | CA | ASN | B | 413 | 0.974 | -23.798 | 21.688 | 1.00 | 36.68 |
| | ATOM | 2796 | CB | ASN | B | 413 | 1.170 | -25.035 | 22.570 | 1.00 | 37.54 |
| | ATOM | 2797 | CG | ASN | B | 413 | 2.017 | -26.100 | 21.901 | 1.00 | 43.56 |
| 25 | ATOM | 2798 | OD1 | ASN | B | 413 | 2.309 | -26.022 | 20.704 | 1.00 | 46.11 |
| | ATOM | 2799 | ND2 | ASN | B | 413 | 2.418 | -27.104 | 22.671 | 1.00 | 47.04 |
| | ATOM | 2800 | C | ASN | B | 413 | -0.383 | -23.168 | 21.982 | 1.00 | 34.01 |
| | ATOM | 2801 | O | ASN | B | 413 | -1.349 | -23.372 | 21.247 | 1.00 | 32.43 |
| | ATOM | 2802 | N | GLN | B | 414 | -0.447 | -22.397 | 23.063 | 1.00 | 32.85 |
| 30 | ATOM | 2803 | CA | GLN | B | 414 | -1.685 | -21.741 | 23.449 | 1.00 | 31.91 |
| | ATOM | 2804 | CB | GLN | B | 414 | -1.558 | -21.172 | 24.863 | 1.00 | 33.17 |
| | ATOM | 2805 | CG | GLN | B | 414 | -1.528 | -22.242 | 25.948 | 1.00 | 32.31 |
| | ATOM | 2806 | CD | GLN | B | 414 | -1.293 | -21.667 | 27.327 | 1.00 | 34.63 |
| | ATOM | 2807 | OE1 | GLN | B | 414 | -0.176 | -21.277 | 27.666 | 1.00 | 33.23 |
| 35 | ATOM | 2808 | NE2 | GLN | B | 414 | -2.349 | -21.606 | 28.131 | 1.00 | 34.56 |
| | ATOM | 2809 | C | GLN | B | 414 | -2.052 | -20.638 | 22.463 | 1.00 | 29.57 |
| | ATOM | 2810 | O | GLN | B | 414 | -3.195 | -20.204 | 22.409 | 1.00 | 31.32 |
| | ATOM | 2811 | N | GLY | B | 415 | -1.077 | -20.190 | 21.682 | 1.00 | 30.96 |
| | ATOM | 2812 | CA | GLY | B | 415 | -1.350 | -19.160 | 20.697 | 1.00 | 34.27 |
| 40 | ATOM | 2813 | C | GLY | B | 415 | -2.184 | -19.725 | 19.562 | 1.00 | 35.27 |
| | ATOM | 2814 | O | GLY | B | 415 | -2.918 | -19.000 | 18.887 | 1.00 | 33.20 |
| | ATOM | 2815 | N | LYS | B | 416 | -2.070 | -21.031 | 19.354 | 1.00 | 35.28 |
| | ATOM | 2816 | CA | LYS | B | 416 | -2.819 | -21.707 | 18.299 | 1.00 | 38.26 |
| | ATOM | 2817 | CB | LYS | B | 416 | -2.398 | -23.177 | 18.201 | 1.00 | 38.00 |
| 45 | ATOM | 2818 | CG | LYS | B | 416 | -0.973 | -23.407 | 17.736 | 1.00 | 40.05 |
| | ATOM | 2819 | CD | LYS | B | 416 | -0.405 | -24.668 | 18.369 | 1.00 | 44.10 |
| | ATOM | 2820 | CE | LYS | B | 416 | 0.306 | -25.541 | 17.346 | 1.00 | 41.85 |
| | ATOM | 2821 | NZ | LYS | B | 416 | 1.286 | -24.760 | 16.542 | 1.00 | 45.63 |
| | ATOM | 2822 | C | LYS | B | 416 | -4.321 | -21.645 | 18.559 | 1.00 | 36.93 |
| 50 | ATOM | 2823 | O | LYS | B | 416 | -5.121 | -21.790 | 17.638 | 1.00 | 38.36 |
| | ATOM | 2824 | N | CYS | B | 417 | -4.698 | -21.430 | 19.817 | 1.00 | 37.10 |
| | ATOM | 2825 | CA | CYS | B | 417 | -6.106 | -21.371 | 20.196 | 1.00 | 36.46 |
| | ATOM | 2826 | CB | CYS | B | 417 | -6.218 | -21.226 | 21.717 | 1.00 | 39.01 |
| | ATOM | 2827 | SG | CYS | B | 417 | -5.674 | -22.710 | 22.612 | 1.00 | 43.81 |
| 55 | ATOM | 2828 | C | CYS | B | 417 | -6.899 | -20.277 | 19.491 | 1.00 | 35.19 |
| | ATOM | 2829 | O | CYS | B | 417 | -8.127 | -20.296 | 19.485 | 1.00 | 33.92 |
| | ATOM | 2830 | N | VAL | B | 418 | -6.195 | -19.316 | 18.906 | 1.00 | 36.04 |
| | ATOM | 2831 | CA | VAL | B | 418 | -6.838 | -18.236 | 18.163 | 1.00 | 34.59 |
| | ATOM | 2832 | CB | VAL | B | 418 | -6.525 | -16.850 | 18.775 | 1.00 | 34.87 |
| 60 | ATOM | 2833 | CG1 | VAL | B | 418 | -6.831 | -15.763 | 17.765 | 1.00 | 35.32 |
| | ATOM | 2834 | CG2 | VAL | B | 418 | -7.350 | -16.630 | 20.036 | 1.00 | 33.65 |
| | ATOM | 2835 | C | VAL | B | 418 | -6.241 | -18.317 | 16.764 | 1.00 | 34.17 |
| | ATOM | 2836 | O | VAL | B | 418 | -5.020 | -18.323 | 16.611 | 1.00 | 32.73 |

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|----|------|------|-----|-----|---|-----|---------|---------|--------|------|-------|
| 5 | ATOM | 2837 | N | GLU | B | 419 | -7.084 | -18.388 | 15.740 | 1.00 | 33.44 |
| | ATOM | 2838 | CA | GLU | B | 419 | -6.554 | -18.500 | 14.390 | 1.00 | 34.52 |
| | ATOM | 2839 | CB | GLU | B | 419 | -7.681 | -18.722 | 13.380 | 1.00 | 36.21 |
| | ATOM | 2840 | CG | GLU | B | 419 | -8.597 | -17.538 | 13.166 | 1.00 | 44.19 |
| | ATOM | 2841 | CD | GLU | B | 419 | -9.477 | -17.723 | 11.946 | 1.00 | 48.47 |
| 10 | ATOM | 2842 | OE1 | GLU | B | 419 | -9.157 | -18.605 | 11.119 | 1.00 | 51.04 |
| | ATOM | 2843 | OE2 | GLU | B | 419 | -10.484 | -16.993 | 11.813 | 1.00 | 48.91 |
| | ATOM | 2844 | C | GLU | B | 419 | -5.717 | -17.289 | 13.997 | 1.00 | 32.89 |
| | ATOM | 2845 | O | GLU | B | 419 | -6.156 | -16.144 | 14.123 | 1.00 | 31.09 |
| | ATOM | 2846 | N | GLY | B | 420 | -4.501 | -17.562 | 13.535 | 1.00 | 32.84 |
| 15 | ATOM | 2847 | CA | GLY | B | 420 | -3.594 | -16.506 | 13.122 | 1.00 | 34.37 |
| | ATOM | 2848 | C | GLY | B | 420 | -2.722 | -15.955 | 14.240 | 1.00 | 35.30 |
| | ATOM | 2849 | O | GLY | B | 420 | -1.745 | -15.246 | 13.975 | 1.00 | 35.94 |
| | ATOM | 2850 | N | MET | B | 421 | -3.052 | -16.285 | 15.486 | 1.00 | 30.08 |
| | ATOM | 2851 | CA | MET | B | 421 | -2.289 | -15.780 | 16.625 | 1.00 | 29.22 |
| 20 | ATOM | 2852 | CB | MET | B | 421 | -3.108 | -15.922 | 17.914 | 1.00 | 22.54 |
| | ATOM | 2853 | CG | MET | B | 421 | -2.469 | -15.270 | 19.124 | 1.00 | 23.82 |
| | ATOM | 2854 | SD | MET | B | 421 | -2.124 | -13.494 | 18.872 | 1.00 | 28.40 |
| | ATOM | 2855 | CE | MET | B | 421 | -3.697 | -12.800 | 19.233 | 1.00 | 24.67 |
| | ATOM | 2856 | C | MET | B | 421 | -0.912 | -16.416 | 16.821 | 1.00 | 29.67 |
| 25 | ATOM | 2857 | O | MET | B | 421 | 0.022 | -15.751 | 17.269 | 1.00 | 29.76 |
| | ATOM | 2858 | N | VAL | B | 422 | -0.766 | -17.694 | 16.484 | 1.00 | 30.63 |
| | ATOM | 2859 | CA | VAL | B | 422 | 0.524 | -18.338 | 16.675 | 1.00 | 29.90 |
| | ATOM | 2860 | CB | VAL | B | 422 | 0.482 | -19.835 | 16.273 | 1.00 | 35.74 |
| | ATOM | 2861 | CG1 | VAL | B | 422 | 0.514 | -19.992 | 14.753 | 1.00 | 37.64 |
| 30 | ATOM | 2862 | CG2 | VAL | B | 422 | 1.659 | -20.555 | 16.897 | 1.00 | 31.68 |
| | ATOM | 2863 | C | VAL | B | 422 | 1.669 | -17.640 | 15.935 | 1.00 | 28.64 |
| | ATOM | 2864 | O | VAL | B | 422 | 2.788 | -17.571 | 16.441 | 1.00 | 26.15 |
| | ATOM | 2865 | N | GLU | B | 423 | 1.402 | -17.113 | 14.747 | 1.00 | 28.70 |
| | ATOM | 2866 | CA | GLU | B | 423 | 2.454 | -16.435 | 13.997 | 1.00 | 31.34 |
| 35 | ATOM | 2867 | CB | GLU | B | 423 | 1.963 | -16.050 | 12.596 | 1.00 | 36.21 |
| | ATOM | 2868 | CG | GLU | B | 423 | 0.502 | -16.376 | 12.325 | 1.00 | 45.83 |
| | ATOM | 2869 | CD | GLU | B | 423 | 0.250 | -17.865 | 12.144 | 1.00 | 46.71 |
| | ATOM | 2870 | OE1 | GLU | B | 423 | -0.746 | -18.368 | 12.706 | 1.00 | 45.97 |
| | ATOM | 2871 | OE2 | GLU | B | 423 | 1.045 | -18.530 | 11.442 | 1.00 | 50.05 |
| 40 | ATOM | 2872 | C | GLU | B | 423 | 2.928 | -15.186 | 14.744 | 1.00 | 30.57 |
| | ATOM | 2873 | O | GLU | B | 423 | 4.119 | -14.870 | 14.759 | 1.00 | 26.59 |
| | ATOM | 2874 | N | ILE | B | 424 | 2.001 | -14.478 | 15.378 | 1.00 | 26.19 |
| | ATOM | 2875 | CA | ILE | B | 424 | 2.381 | -13.279 | 16.111 | 1.00 | 26.23 |
| | ATOM | 2876 | CB | ILE | B | 424 | 1.134 | -12.435 | 16.452 | 1.00 | 29.33 |
| 45 | ATOM | 2877 | CG2 | ILE | B | 424 | 1.492 | -11.315 | 17.425 | 1.00 | 30.91 |
| | ATOM | 2878 | CG1 | ILE | B | 424 | 0.584 | -11.817 | 15.160 | 1.00 | 29.09 |
| | ATOM | 2879 | CD1 | ILE | B | 424 | -0.895 | -11.514 | 15.187 | 1.00 | 30.51 |
| | ATOM | 2880 | C | ILE | B | 424 | 3.153 | -13.673 | 17.370 | 1.00 | 24.22 |
| | ATOM | 2881 | O | ILE | B | 424 | 4.152 | -13.037 | 17.725 | 1.00 | 21.05 |
| 50 | ATOM | 2882 | N | PHE | B | 425 | 2.708 | -14.746 | 18.023 | 1.00 | 21.71 |
| | ATOM | 2883 | CA | PHE | B | 425 | 3.370 | -15.236 | 19.223 | 1.00 | 18.85 |
| | ATOM | 2884 | CB | PHE | B | 425 | 2.650 | -16.479 | 19.768 | 1.00 | 22.98 |
| | ATOM | 2885 | CG | PHE | B | 425 | 1.580 | -16.183 | 20.795 | 1.00 | 22.17 |
| | ATOM | 2886 | CD1 | PHE | B | 425 | 1.287 | -17.112 | 21.792 | 1.00 | 25.47 |
| 55 | ATOM | 2887 | CD2 | PHE | B | 425 | 0.843 | -15.001 | 20.747 | 1.00 | 26.30 |
| | ATOM | 2888 | CE1 | PHE | B | 425 | 0.273 | -16.871 | 22.724 | 1.00 | 24.33 |
| | ATOM | 2889 | CE2 | PHE | B | 425 | -0.174 | -14.749 | 21.676 | 1.00 | 25.03 |
| | ATOM | 2890 | CZ | PHE | B | 425 | -0.459 | -15.684 | 22.663 | 1.00 | 26.44 |
| | ATOM | 2891 | C | PHE | B | 425 | 4.817 | -15.610 | 18.885 | 1.00 | 20.00 |
| 60 | ATOM | 2892 | O | PHE | B | 425 | 5.741 | -15.292 | 19.636 | 1.00 | 21.15 |
| | ATOM | 2893 | N | ASP | B | 426 | 5.023 | -16.281 | 17.754 | 1.00 | 19.87 |

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 2894 | CA | ASP | B | 426 | 6.378 | -16.685 | 17.377 | 1.00 | 23.20 |
| | ATOM | 2895 | CB | ASP | B | 426 | 6.364 | -17.510 | 16.090 | 1.00 | 26.53 |
| | ATOM | 2896 | CG | ASP | B | 426 | 5.992 | -18.965 | 16.335 | 1.00 | 34.28 |
| | ATOM | 2897 | OD1 | ASP | B | 426 | 6.242 | -19.467 | 17.455 | 1.00 | 35.24 |
| | ATOM | 2898 | OD2 | ASP | B | 426 | 5.448 | -19.600 | 15.409 | 1.00 | 31.49 |
| 10 | ATOM | 2899 | C | ASP | B | 426 | 7.302 | -15.489 | 17.198 | 1.00 | 21.84 |
| | ATOM | 2900 | O | ASP | B | 426 | 8.465 | -15.526 | 17.593 | 1.00 | 21.55 |
| | ATOM | 2901 | N | MET | B | 427 | 6.788 | -14.429 | 16.591 | 1.00 | 20.12 |
| | ATOM | 2902 | CA | MET | B | 427 | 7.597 | -13.234 | 16.382 | 1.00 | 21.02 |
| | ATOM | 2903 | CB | MET | B | 427 | 6.836 | -12.228 | 15.520 | 1.00 | 18.53 |
| 15 | ATOM | 2904 | CG | MET | B | 427 | 6.864 | -12.559 | 14.038 | 1.00 | 27.92 |
| | ATOM | 2905 | SD | MET | B | 427 | 6.011 | -11.341 | 13.024 | 1.00 | 32.84 |
| | ATOM | 2906 | CE | MET | B | 427 | 4.363 | -11.532 | 13.581 | 1.00 | 33.63 |
| | ATOM | 2907 | C | MET | B | 427 | 7.945 | -12.616 | 17.732 | 1.00 | 17.42 |
| | ATOM | 2908 | O | MET | B | 427 | 9.073 | -12.180 | 17.950 | 1.00 | 22.09 |
| 20 | ATOM | 2909 | N | LEU | B | 428 | 6.968 | -12.597 | 18.634 | 1.00 | 20.47 |
| | ATOM | 2910 | CA | LEU | B | 428 | 7.157 | -12.033 | 19.968 | 1.00 | 20.13 |
| | ATOM | 2911 | CB | LEU | B | 428 | 5.812 | -11.964 | 20.706 | 1.00 | 17.58 |
| | ATOM | 2912 | CG | LEU | B | 428 | 4.852 | -10.887 | 20.179 | 1.00 | 18.41 |
| | ATOM | 2913 | CD1 | LEU | B | 428 | 3.443 | -11.155 | 20.687 | 1.00 | 11.95 |
| 25 | ATOM | 2914 | CD2 | LEU | B | 428 | 5.324 | -9.505 | 20.631 | 1.00 | 17.80 |
| | ATOM | 2915 | C | LEU | B | 428 | 8.159 | -12.856 | 20.767 | 1.00 | 20.68 |
| | ATOM | 2916 | O | LEU | B | 428 | 9.028 | -12.305 | 21.445 | 1.00 | 20.45 |
| | ATOM | 2917 | N | LEU | B | 429 | 8.037 | -14.178 | 20.679 | 1.00 | 20.35 |
| | ATOM | 2918 | CA | LEU | B | 429 | 8.938 | -15.082 | 21.382 | 1.00 | 19.82 |
| 30 | ATOM | 2919 | CB | LEU | B | 429 | 8.470 | -16.532 | 21.211 | 1.00 | 23.13 |
| | ATOM | 2920 | CG | LEU | B | 429 | 7.189 | -16.839 | 21.997 | 1.00 | 21.85 |
| | ATOM | 2921 | CD1 | LEU | B | 429 | 6.551 | -18.123 | 21.494 | 1.00 | 25.39 |
| | ATOM | 2922 | CD2 | LEU | B | 429 | 7.537 | -16.944 | 23.475 | 1.00 | 24.91 |
| | ATOM | 2923 | C | LEU | B | 429 | 10.361 | -14.936 | 20.865 | 1.00 | 20.74 |
| 35 | ATOM | 2924 | O | LEU | B | 429 | 11.318 | -14.968 | 21.638 | 1.00 | 21.02 |
| | ATOM | 2925 | N | ALA | B | 430 | 10.495 | -14.770 | 19.554 | 1.00 | 21.40 |
| | ATOM | 2926 | CA | ALA | B | 430 | 11.808 | -14.609 | 18.947 | 1.00 | 22.77 |
| | ATOM | 2927 | CB | ALA | B | 430 | 11.677 | -14.596 | 17.432 | 1.00 | 21.11 |
| | ATOM | 2928 | C | ALA | B | 430 | 12.467 | -13.315 | 19.440 | 1.00 | 22.40 |
| 40 | ATOM | 2929 | O | ALA | B | 430 | 13.670 | -13.277 | 19.713 | 1.00 | 20.62 |
| | ATOM | 2930 | N | THR | B | 431 | 11.670 | -12.258 | 19.567 | 1.00 | 21.09 |
| | ATOM | 2931 | CA | THR | B | 431 | 12.183 | -10.974 | 20.021 | 1.00 | 22.67 |
| | ATOM | 2932 | CB | THR | B | 431 | 11.128 | -9.866 | 19.863 | 1.00 | 23.77 |
| | ATOM | 2933 | OG1 | THR | B | 431 | 10.572 | -9.936 | 18.547 | 1.00 | 23.84 |
| 45 | ATOM | 2934 | CG2 | THR | B | 431 | 11.762 | -8.489 | 20.073 | 1.00 | 21.78 |
| | ATOM | 2935 | C | THR | B | 431 | 12.603 | -11.037 | 21.480 | 1.00 | 21.98 |
| | ATOM | 2936 | O | THR | B | 431 | 13.595 | -10.429 | 21.879 | 1.00 | 19.85 |
| | ATOM | 2937 | N | SER | B | 432 | 11.844 | -11.773 | 22.280 | 1.00 | 24.24 |
| | ATOM | 2938 | CA | SER | B | 432 | 12.169 | -11.906 | 23.693 | 1.00 | 26.96 |
| 50 | ATOM | 2939 | CB | SER | B | 432 | 11.055 | -12.661 | 24.423 | 1.00 | 28.00 |
| | ATOM | 2940 | OG | SER | B | 432 | 11.404 | -12.888 | 25.776 | 1.00 | 30.31 |
| | ATOM | 2941 | C | SER | B | 432 | 13.491 | -12.660 | 23.820 | 1.00 | 27.67 |
| | ATOM | 2942 | O | SER | B | 432 | 14.305 | -12.377 | 24.701 | 1.00 | 23.78 |
| | ATOM | 2943 | N | SER | B | 433 | 13.691 | -13.628 | 22.932 | 1.00 | 29.27 |
| 55 | ATOM | 2944 | CA | SER | B | 433 | 14.914 | -14.421 | 22.928 | 1.00 | 31.96 |
| | ATOM | 2945 | CB | SER | B | 433 | 14.790 | -15.575 | 21.938 | 1.00 | 30.84 |
| | ATOM | 2946 | OG | SER | B | 433 | 14.761 | -16.808 | 22.625 | 1.00 | 38.26 |
| | ATOM | 2947 | C | SER | B | 433 | 16.104 | -13.550 | 22.548 | 1.00 | 31.47 |
| | ATOM | 2948 | O | SER | B | 433 | 17.204 | -13.701 | 23.087 | 1.00 | 28.43 |
| 60 | ATOM | 2949 | N | ARG | B | 434 | 15.878 | -12.641 | 21.607 | 1.00 | 29.55 |
| | ATOM | 2950 | CA | ARG | B | 434 | 16.926 | -11.739 | 21.165 | 1.00 | 29.40 |

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|----|------|------|-----|------|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 2951 | CB | ARG | B | 434 | 16.437 | -10.912 | 19.977 | 1.00 | 31.56 |
| | ATOM | 2952 | CG | ARG | B | 434 | 17.428 | -9.868 | 19.493 | 1.00 | 36.76 |
| | ATOM | 2953 | CD | ARG | B | 434 | 18.694 | -10.502 | 18.919 | 1.00 | 37.76 |
| | ATOM | 2954 | NE | ARG | B | 434 | 19.654 | -9.479 | 18.516 | 1.00 | 39.50 |
| | ATOM | 2955 | CZ | ARG | B | 434 | 20.965 | -9.673 | 18.418 | 1.00 | 44.17 |
| 10 | ATOM | 2956 | NH1 | ARG | B | 434 | 21.492 | -10.861 | 18.696 | 1.00 | 43.17 |
| | ATOM | 2957 | NH2 | ARG | B | 434 | 21.750 | -8.671 | 18.048 | 1.00 | 43.05 |
| | ATOM | 2958 | C | ARG | B | 434 | 17.328 | -10.827 | 22.326 | 1.00 | 29.15 |
| | ATOM | 2959 | O | ARG | B | 434 | 18.515 | -10.612 | 22.569 | 1.00 | 28.82 |
| | ATOM | 2960 | N | PHE | B | 435 | 16.337 | -10.297 | 23.039 | 1.00 | 24.88 |
| 15 | ATOM | 2961 | CA | PHE | B | 435 | 16.600 | -9.422 | 24.186 | 1.00 | 25.74 |
| | ATOM | 2962 | CB | PHE | B | 435 | 15.278 | -8.972 | 24.825 | 1.00 | 26.53 |
| | ATOM | 2963 | CG | PHE | B | 435 | 14.656 | -7.758 | 24.183 | 1.00 | 30.94 |
| | ATOM | 2964 | CD1 | PHE | B | 435 | 15.118 | -7.271 | 22.966 | 1.00 | 32.65 |
| | ATOM | 2965 | CD2 | PHE | B | 435 | 13.592 | -7.108 | 24.797 | 1.00 | 33.60 |
| 20 | ATOM | 2966 | CE1 | PHE | B | 435 | 14.529 | -6.155 | 22.372 | 1.00 | 36.84 |
| | ATOM | 2967 | CE2 | PHE | B | 435 | 12.997 | -5.989 | 24.208 | 1.00 | 34.96 |
| | ATOM | 2968 | CZ | PHE | B | 435 | 13.468 | -5.516 | 22.995 | 1.00 | 31.64 |
| | ATOM | 2969 | C | PHE | B | 435 | 17.426 | -10.184 | 25.233 | 1.00 | 25.39 |
| | ATOM | 2970 | O | PHE | B | 435 | 18.414 | -9.675 | 25.764 | 1.00 | 22.59 |
| 25 | ATOM | 2971 | N | ARG | B | 436 | 16.999 | -11.405 | 25.528 | 1.00 | 24.58 |
| | ATOM | 2972 | CA | ARG | B | 436 | 17.675 | -12.253 | 26.503 | 1.00 | 30.25 |
| | ATOM | 2973 | CB | ARG | B | 436 | 16.898 | -13.569 | 26.662 | 1.00 | 33.32 |
| | ATOM | 2974 | CG | ARG | B | 436 | 17.232 | -14.358 | 27.915 | 1.00 | 38.17 |
| | ATOM | 2975 | CD | ARG | B | 436 | 16.135 | -15.367 | 28.260 | 1.00 | 37.27 |
| 30 | ATOM | 2976 | NE | ARG | B | 436 | 15.646 | -16.085 | 27.086 | 1.00 | 43.92 |
| | ATOM | 2977 | CZ | ARG | B | 436 | 14.433 | -15.923 | 26.557 | 1.00 | 46.68 |
| | ATOM | 2978 | NH1 | ARG | B | 436 | 13.578 | -15.061 | 27.097 | 1.00 | 45.59 |
| | ATOM | 2979 | NH2 | ARG | B | 436 | 14.074 | -16.620 | 25.486 | 1.00 | 46.25 |
| | ATOM | 2980 | C | ARG | B | 436 | 19.110 | -12.531 | 26.048 | 1.00 | 29.82 |
| 35 | ATOM | 2981 | O | ARG | B | 436 | 20.057 | -12.397 | 26.823 | 1.00 | 28.76 |
| | ATOM | 2982 | N | AMET | B | 437 | 19.269 | -12.921 | 24.789 | 0.50 | 30.27 |
| | ATOM | 2983 | N | BMET | B | 437 | 19.252 | -12.906 | 24.781 | 0.50 | 31.41 |
| | ATOM | 2984 | CA | AMET | B | 437 | 20.591 | -13.212 | 24.253 | 0.50 | 31.98 |
| | ATOM | 2985 | CA | BMET | B | 437 | 20.547 | -13.206 | 24.183 | 0.50 | 33.77 |
| 40 | ATOM | 2986 | CB | AMET | B | 437 | 20.489 | -13.646 | 22.788 | 0.50 | 31.34 |
| | ATOM | 2987 | CB | BMET | B | 437 | 20.348 | -13.595 | 22.714 | 0.50 | 35.88 |
| | ATOM | 2988 | CG | AMET | B | 437 | 20.179 | -15.127 | 22.592 | 0.50 | 33.62 |
| | ATOM | 2989 | CG | BMET | B | 437 | 21.605 | -13.594 | 21.861 | 0.50 | 40.47 |
| | ATOM | 2990 | SD | AMET | B | 437 | 20.354 | -16.099 | 24.109 | 0.50 | 35.21 |
| 45 | ATOM | 2991 | SD | BMET | B | 437 | 21.247 | -13.937 | 20.115 | 0.50 | 46.79 |
| | ATOM | 2992 | CE | AMET | B | 437 | 22.155 | -16.194 | 24.259 | 0.50 | 33.20 |
| | ATOM | 2993 | CE | BMET | B | 437 | 21.837 | -15.632 | 19.976 | 0.50 | 43.22 |
| | ATOM | 2994 | C | AMET | B | 437 | 21.498 | -11.993 | 24.366 | 0.50 | 33.33 |
| | ATOM | 2995 | C | BMET | B | 437 | 21.487 | -12.005 | 24.289 | 0.50 | 34.45 |
| 50 | ATOM | 2996 | O | AMET | B | 437 | 22.702 | -12.123 | 24.594 | 0.50 | 33.54 |
| | ATOM | 2997 | O | BMET | B | 437 | 22.699 | -12.162 | 24.438 | 0.50 | 34.43 |
| | ATOM | 2998 | N | MET | B | 438 | 20.913 | -10.809 | 24.215 | 1.00 | 32.07 |
| | ATOM | 2999 | CA | MET | B | 438 | 21.674 | -9.560 | 24.298 | 1.00 | 32.48 |
| | ATOM | 3000 | CB | MET | B | 438 | 20.930 | -8.437 | 23.578 | 1.00 | 29.74 |
| 55 | ATOM | 3001 | CG | MET | B | 438 | 21.161 | -8.364 | 22.093 | 1.00 | 36.73 |
| | ATOM | 3002 | SD | MET | B | 438 | 20.425 | -6.849 | 21.462 | 1.00 | 38.21 |
| | ATOM | 3003 | CE | MET | B | 438 | 21.693 | -5.657 | 21.943 | 1.00 | 35.91 |
| | ATOM | 3004 | C | MET | B | 438 | 21.877 | -9.122 | 25.738 | 1.00 | 28.81 |
| | ATOM | 3005 | O | MET | B | 438 | 22.686 | -8.240 | 26.013 | 1.00 | 30.13 |
| 60 | ATOM | 3006 | N | ASN | B | 439 | 21.120 | -9.721 | 26.646 | 1.00 | 27.14 |
| | ATOM | 3007 | CA | ASN | B | 439 | 21.199 | -9.359 | 28.038 | 1.00 | 27.34 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3008 | CB | ASN | B | 439 | 22.592 | -9.524 | 28.598 | 1.00 | 34.85 |
| | ATOM | 3009 | CG | ASN | B | 439 | 22.624 | -9.480 | 30.080 | 1.00 | 38.58 |
| | ATOM | 3010 | OD1 | ASN | B | 439 | 21.584 | -9.620 | 30.724 | 1.00 | 42.99 |
| | ATOM | 3011 | ND2 | ASN | B | 439 | 23.801 | -9.260 | 30.666 | 1.00 | 41.14 |
| 10 | ATOM | 3012 | C | ASN | B | 439 | 20.745 | -7.903 | 28.212 | 1.00 | 26.24 |
| | ATOM | 3013 | O | ASN | B | 439 | 21.396 | -7.106 | 28.891 | 1.00 | 19.76 |
| | ATOM | 3014 | N | LEU | B | 440 | 19.625 | -7.564 | 27.573 | 1.00 | 24.90 |
| | ATOM | 3015 | CA | LEU | B | 440 | 19.061 | -6.214 | 27.633 | 1.00 | 25.04 |
| 15 | ATOM | 3016 | CB | LEU | B | 440 | 17.761 | -6.157 | 26.818 | 1.00 | 22.36 |
| | ATOM | 3017 | CG | LEU | B | 440 | 17.087 | -4.786 | 26.740 | 1.00 | 26.33 |
| | ATOM | 3018 | CD1 | LEU | B | 440 | 17.958 | -3.843 | 25.923 | 1.00 | 28.33 |
| | ATOM | 3019 | CD2 | LEU | B | 440 | 15.704 | -4.914 | 26.111 | 1.00 | 24.81 |
| 20 | ATOM | 3020 | C | LEU | B | 440 | 18.782 | -5.785 | 29.074 | 1.00 | 24.71 |
| | ATOM | 3021 | O | LEU | B | 440 | 18.131 | -6.504 | 29.830 | 1.00 | 26.96 |
| | ATOM | 3022 | N | GLN | B | 441 | 19.268 | -4.609 | 29.452 | 1.00 | 25.54 |
| | ATOM | 3023 | CA | GLN | B | 441 | 19.060 | -4.099 | 30.807 | 1.00 | 25.82 |
| 25 | ATOM | 3024 | CB | GLN | B | 441 | 20.250 | -3.231 | 31.234 | 1.00 | 30.41 |
| | ATOM | 3025 | CG | GLN | B | 441 | 21.572 | -3.956 | 31.228 | 1.00 | 30.50 |
| | ATOM | 3026 | CD | GLN | B | 441 | 21.610 | -5.028 | 32.279 | 1.00 | 32.75 |
| | ATOM | 3027 | OE1 | GLN | B | 441 | 21.539 | -4.772 | 33.473 | 1.00 | 36.52 |
| 30 | ATOM | 3028 | NE2 | GLN | B | 441 | 21.703 | -6.288 | 31.823 | 1.00 | 31.09 |
| | ATOM | 3029 | C | GLN | B | 441 | 17.789 | -3.265 | 30.883 | 1.00 | 26.93 |
| | ATOM | 3030 | O | GLN | B | 441 | 17.303 | -2.768 | 29.866 | 1.00 | 25.40 |
| | ATOM | 3031 | N | GLY | B | 442 | 17.266 | -3.105 | 32.096 | 1.00 | 24.56 |
| 35 | ATOM | 3032 | CA | GLY | B | 442 | 16.058 | -2.327 | 32.293 | 1.00 | 22.82 |
| | ATOM | 3033 | C | GLY | B | 442 | 16.217 | -0.873 | 31.885 | 1.00 | 24.19 |
| | ATOM | 3034 | O | GLY | B | 442 | 15.290 | -0.279 | 31.341 | 1.00 | 20.21 |
| | ATOM | 3035 | N | GLU | B | 443 | 17.387 | -0.293 | 32.141 | 1.00 | 22.92 |
| 40 | ATOM | 3036 | CA | GLU | B | 443 | 17.635 | 1.102 | 31.778 | 1.00 | 23.33 |
| | ATOM | 3037 | CB | GLU | B | 443 | 18.960 | 1.590 | 32.378 | 1.00 | 24.26 |
| | ATOM | 3038 | CG | GLU | B | 443 | 19.005 | 1.525 | 33.895 | 1.00 | 32.31 |
| | ATOM | 3039 | CD | GLU | B | 443 | 19.701 | 0.270 | 34.402 | 1.00 | 37.68 |
| 45 | ATOM | 3040 | OE1 | GLU | B | 443 | 19.343 | -0.841 | 33.948 | 1.00 | 35.23 |
| | ATOM | 3041 | OE2 | GLU | B | 443 | 20.607 | 0.394 | 35.252 | 1.00 | 42.47 |
| | ATOM | 3042 | C | GLU | B | 443 | 17.662 | 1.278 | 30.262 | 1.00 | 23.08 |
| | ATOM | 3043 | O | GLU | B | 443 | 17.265 | 2.328 | 29.747 | 1.00 | 21.80 |
| 50 | ATOM | 3044 | N | GLU | B | 444 | 18.128 | 0.253 | 29.552 | 1.00 | 21.16 |
| | ATOM | 3045 | CA | GLU | B | 444 | 18.182 | 0.302 | 28.093 | 1.00 | 22.60 |
| | ATOM | 3046 | CB | GLU | B | 444 | 19.046 | -0.834 | 27.545 | 1.00 | 20.89 |
| | ATOM | 3047 | CG | GLU | B | 444 | 20.545 | -0.617 | 27.705 | 1.00 | 23.24 |
| 55 | ATOM | 3048 | CD | GLU | B | 444 | 21.340 | -1.869 | 27.393 | 1.00 | 22.11 |
| | ATOM | 3049 | OE1 | GLU | B | 444 | 20.817 | -2.978 | 27.629 | 1.00 | 20.89 |
| | ATOM | 3050 | OE2 | GLU | B | 444 | 22.488 | -1.746 | 26.914 | 1.00 | 25.49 |
| | ATOM | 3051 | C | GLU | B | 444 | 16.758 | 0.155 | 27.552 | 1.00 | 21.06 |
| 60 | ATOM | 3052 | O | GLU | B | 444 | 16.377 | 0.822 | 26.597 | 1.00 | 23.73 |
| | ATOM | 3053 | N | PHE | B | 445 | 15.987 | -0.730 | 28.176 | 1.00 | 19.01 |
| | ATOM | 3054 | CA | PHE | B | 445 | 14.600 | -0.969 | 27.792 | 1.00 | 19.44 |
| | ATOM | 3055 | CB | PHE | B | 445 | 13.989 | -2.067 | 28.675 | 1.00 | 18.12 |
| 65 | ATOM | 3056 | CG | PHE | B | 445 | 12.483 | -2.055 | 28.709 | 1.00 | 18.13 |
| | ATOM | 3057 | CD1 | PHE | B | 445 | 11.746 | -2.386 | 27.575 | 1.00 | 18.34 |
| | ATOM | 3058 | CD2 | PHE | B | 445 | 11.802 | -1.694 | 29.872 | 1.00 | 16.59 |
| | ATOM | 3059 | CE1 | PHE | B | 445 | 10.346 | -2.359 | 27.592 | 1.00 | 17.15 |
| 70 | ATOM | 3060 | CE2 | PHE | B | 445 | 10.406 | -1.662 | 29.903 | 1.00 | 21.99 |
| | ATOM | 3061 | CZ | PHE | B | 445 | 9.674 | -1.997 | 28.755 | 1.00 | 16.01 |
| | ATOM | 3062 | C | PHE | B | 445 | 13.758 | 0.304 | 27.888 | 1.00 | 15.87 |
| | ATOM | 3063 | O | PHE | B | 445 | 13.008 | 0.617 | 26.966 | 1.00 | 20.27 |
| | ATOM | 3064 | N | VAL | B | 446 | 13.872 | 1.044 | 28.986 | 1.00 | 15.90 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3065 | CA | VAL | B | 446 | 13.074 | 2.269 | 29.112 | 1.00 | 16.78 |
| | ATOM | 3066 | CB | VAL | B | 446 | 13.165 | 2.895 | 30.531 | 1.00 | 18.32 |
| | ATOM | 3067 | CG1 | VAL | B | 446 | 12.574 | 1.923 | 31.551 | 1.00 | 21.14 |
| | ATOM | 3068 | CG2 | VAL | B | 446 | 14.598 | 3.251 | 30.879 | 1.00 | 21.04 |
| | ATOM | 3069 | C | VAL | B | 446 | 13.450 | 3.295 | 28.051 | 1.00 | 17.91 |
| 10 | ATOM | 3070 | O | VAL | B | 446 | 12.596 | 4.028 | 27.561 | 1.00 | 19.37 |
| | ATOM | 3071 | N | CYS | B | 447 | 14.723 | 3.335 | 27.674 | 1.00 | 18.81 |
| | ATOM | 3072 | CA | CYS | B | 447 | 15.161 | 4.255 | 26.635 | 1.00 | 17.34 |
| | ATOM | 3073 | CB | CYS | B | 447 | 16.682 | 4.224 | 26.512 | 1.00 | 19.33 |
| | ATOM | 3074 | SG | CYS | B | 447 | 17.538 | 5.134 | 27.798 | 1.00 | 23.60 |
| 15 | ATOM | 3075 | C | CYS | B | 447 | 14.537 | 3.826 | 25.301 | 1.00 | 18.09 |
| | ATOM | 3076 | O | CYS | B | 447 | 13.988 | 4.643 | 24.563 | 1.00 | 17.52 |
| | ATOM | 3077 | N | LEU | B | 448 | 14.623 | 2.533 | 25.006 | 1.00 | 15.60 |
| | ATOM | 3078 | CA | LEU | B | 448 | 14.072 | 1.994 | 23.767 | 1.00 | 16.67 |
| | ATOM | 3079 | CB | LEU | B | 448 | 14.328 | 0.490 | 23.684 | 1.00 | 14.82 |
| 20 | ATOM | 3080 | CG | LEU | B | 448 | 15.730 | 0.009 | 23.301 | 1.00 | 23.57 |
| | ATOM | 3081 | CD1 | LEU | B | 448 | 15.722 | -1.522 | 23.169 | 1.00 | 21.61 |
| | ATOM | 3082 | CD2 | LEU | B | 448 | 16.167 | 0.658 | 21.986 | 1.00 | 18.92 |
| | ATOM | 3083 | C | LEU | B | 448 | 12.573 | 2.249 | 23.652 | 1.00 | 15.98 |
| | ATOM | 3084 | O | LEU | B | 448 | 12.078 | 2.633 | 22.590 | 1.00 | 18.91 |
| 25 | ATOM | 3085 | N | LYS | B | 449 | 11.849 | 2.037 | 24.745 | 1.00 | 17.94 |
| | ATOM | 3086 | CA | LYS | B | 449 | 10.405 | 2.232 | 24.733 | 1.00 | 16.66 |
| | ATOM | 3087 | CB | LYS | B | 449 | 9.796 | 1.745 | 26.047 | 1.00 | 16.45 |
| | ATOM | 3088 | CG | LYS | B | 449 | 8.285 | 1.861 | 26.115 | 1.00 | 16.12 |
| | ATOM | 3089 | CD | LYS | B | 449 | 7.730 | 0.952 | 27.193 | 1.00 | 19.09 |
| 30 | ATOM | 3090 | CE | LYS | B | 449 | 8.201 | 1.380 | 28.580 | 1.00 | 17.04 |
| | ATOM | 3091 | NZ | LYS | B | 449 | 7.159 | 1.088 | 29.593 | 1.00 | 17.25 |
| | ATOM | 3092 | C | LYS | B | 449 | 10.058 | 3.696 | 24.486 | 1.00 | 18.78 |
| | ATOM | 3093 | O | LYS | B | 449 | 9.103 | 3.996 | 23.769 | 1.00 | 14.84 |
| | ATOM | 3094 | N | SER | B | 450 | 10.837 | 4.610 | 25.059 | 1.00 | 14.50 |
| 35 | ATOM | 3095 | CA | SER | B | 450 | 10.591 | 6.032 | 24.849 | 1.00 | 17.11 |
| | ATOM | 3096 | CB | SER | B | 450 | 11.440 | 6.866 | 25.815 | 1.00 | 21.20 |
| | ATOM | 3097 | OG | SER | B | 450 | 10.859 | 6.868 | 27.108 | 1.00 | 30.66 |
| | ATOM | 3098 | C | SER | B | 450 | 10.921 | 6.418 | 23.405 | 1.00 | 17.84 |
| | ATOM | 3099 | O | SER | B | 450 | 10.279 | 7.292 | 22.821 | 1.00 | 18.82 |
| 40 | ATOM | 3100 | N | ILE | B | 451 | 11.926 | 5.768 | 22.828 | 1.00 | 16.88 |
| | ATOM | 3101 | CA | ILE | B | 451 | 12.305 | 6.063 | 21.450 | 1.00 | 17.11 |
| | ATOM | 3102 | CB | ILE | B | 451 | 13.564 | 5.268 | 21.025 | 1.00 | 16.69 |
| | ATOM | 3103 | CG2 | ILE | B | 451 | 13.724 | 5.298 | 19.505 | 1.00 | 19.31 |
| | ATOM | 3104 | CG1 | ILE | B | 451 | 14.804 | 5.897 | 21.676 | 1.00 | 18.96 |
| 45 | ATOM | 3105 | CD1 | ILE | B | 451 | 16.083 | 5.130 | 21.431 | 1.00 | 18.98 |
| | ATOM | 3106 | C | ILE | B | 451 | 11.142 | 5.711 | 20.527 | 1.00 | 18.09 |
| | ATOM | 3107 | O | ILE | B | 451 | 10.820 | 6.464 | 19.608 | 1.00 | 17.07 |
| | ATOM | 3108 | N | ILE | B | 452 | 10.505 | 4.571 | 20.786 | 1.00 | 18.13 |
| | ATOM | 3109 | CA | ILE | B | 452 | 9.373 | 4.137 | 19.976 | 1.00 | 16.77 |
| 50 | ATOM | 3110 | CB | ILE | B | 452 | 8.804 | 2.775 | 20.477 | 1.00 | 17.40 |
| | ATOM | 3111 | CG2 | ILE | B | 452 | 7.464 | 2.496 | 19.831 | 1.00 | 14.33 |
| | ATOM | 3112 | CG1 | ILE | B | 452 | 9.763 | 1.635 | 20.107 | 1.00 | 15.36 |
| | ATOM | 3113 | CD1 | ILE | B | 452 | 9.449 | 0.323 | 20.805 | 1.00 | 17.76 |
| | ATOM | 3114 | C | ILE | B | 452 | 8.271 | 5.195 | 20.024 | 1.00 | 17.47 |
| 55 | ATOM | 3115 | O | ILE | B | 452 | 7.733 | 5.586 | 18.992 | 1.00 | 16.50 |
| | ATOM | 3116 | N | LEU | B | 453 | 7.943 | 5.665 | 21.222 | 1.00 | 16.06 |
| | ATOM | 3117 | CA | LEU | B | 453 | 6.903 | 6.680 | 21.374 | 1.00 | 17.17 |
| | ATOM | 3118 | CB | LEU | B | 453 | 6.736 | 7.061 | 22.850 | 1.00 | 16.23 |
| | ATOM | 3119 | CG | LEU | B | 453 | 5.792 | 8.228 | 23.163 | 1.00 | 17.60 |
| 60 | ATOM | 3120 | CD1 | LEU | B | 453 | 4.388 | 7.881 | 22.704 | 1.00 | 16.94 |
| | ATOM | 3121 | CD2 | LEU | B | 453 | 5.816 | 8.538 | 24.667 | 1.00 | 17.17 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3122 | C | LEU | B | 453 | 7.198 | 7.941 | 20.566 | 1.00 | 19.33 |
| | ATOM | 3123 | O | LEU | B | 453 | 6.320 | 8.458 | 19.879 | 1.00 | 21.37 |
| | ATOM | 3124 | N | LEU | B | 454 | 8.434 | 8.428 | 20.636 | 1.00 | 17.68 |
| | ATOM | 3125 | CA | LEU | B | 454 | 8.789 | 9.653 | 19.933 | 1.00 | 20.93 |
| | ATOM | 3126 | CB | LEU | B | 454 | 9.959 | 10.347 | 20.653 | 1.00 | 24.33 |
| 10 | ATOM | 3127 | CG | LEU | B | 454 | 9.735 | 10.699 | 22.130 | 1.00 | 26.16 |
| | ATOM | 3128 | CD1 | LEU | B | 454 | 11.046 | 11.170 | 22.749 | 1.00 | 24.82 |
| | ATOM | 3129 | CD2 | LEU | B | 454 | 8.658 | 11.777 | 22.259 | 1.00 | 23.79 |
| | ATOM | 3130 | C | LEU | B | 454 | 9.120 | 9.494 | 18.449 | 1.00 | 20.75 |
| | ATOM | 3131 | O | LEU | B | 454 | 8.941 | 10.431 | 17.673 | 1.00 | 21.33 |
| 15 | ATOM | 3132 | N | ASN | B | 455 | 9.566 | 8.311 | 18.042 | 1.00 | 20.54 |
| | ATOM | 3133 | CA | ASN | B | 455 | 9.951 | 8.093 | 16.651 | 1.00 | 19.46 |
| | ATOM | 3134 | CB | ASN | B | 455 | 11.147 | 7.149 | 16.584 | 1.00 | 18.58 |
| | ATOM | 3135 | CG | ASN | B | 455 | 11.576 | 6.871 | 15.161 | 1.00 | 17.64 |
| | ATOM | 3136 | OD1 | ASN | B | 455 | 12.106 | 7.749 | 14.496 | 1.00 | 18.40 |
| 20 | ATOM | 3137 | ND2 | ASN | B | 455 | 11.343 | 5.648 | 14.686 | 1.00 | 15.06 |
| | ATOM | 3138 | C | ASN | B | 455 | 8.925 | 7.580 | 15.655 | 1.00 | 22.77 |
| | ATOM | 3139 | O | ASN | B | 455 | 8.790 | 8.127 | 14.564 | 1.00 | 21.94 |
| | ATOM | 3140 | N | SER | B | 456 | 8.224 | 6.514 | 16.023 | 1.00 | 25.90 |
| | ATOM | 3141 | CA | SER | B | 456 | 7.260 | 5.873 | 15.135 | 1.00 | 24.76 |
| 25 | ATOM | 3142 | CB | SER | B | 456 | 6.402 | 4.894 | 15.939 | 1.00 | 26.91 |
| | ATOM | 3143 | OG | SER | B | 456 | 7.212 | 3.818 | 16.390 | 1.00 | 26.24 |
| | ATOM | 3144 | C | SER | B | 456 | 6.385 | 6.774 | 14.272 | 1.00 | 26.52 |
| | ATOM | 3145 | O | SER | B | 456 | 6.323 | 6.588 | 13.055 | 1.00 | 29.22 |
| | ATOM | 3146 | N | GLY | B | 457 | 5.716 | 7.750 | 14.872 | 1.00 | 22.07 |
| 30 | ATOM | 3147 | CA | GLY | B | 457 | 4.879 | 8.627 | 14.076 | 1.00 | 25.19 |
| | ATOM | 3148 | C | GLY | B | 457 | 5.510 | 9.973 | 13.765 | 1.00 | 28.59 |
| | ATOM | 3149 | O | GLY | B | 457 | 4.851 | 10.850 | 13.214 | 1.00 | 28.31 |
| | ATOM | 3150 | N | VAL | B | 458 | 6.789 | 10.130 | 14.092 | 1.00 | 31.65 |
| | ATOM | 3151 | CA | VAL | B | 458 | 7.486 | 11.396 | 13.879 | 1.00 | 38.50 |
| 35 | ATOM | 3152 | CB | VAL | B | 458 | 8.950 | 11.310 | 14.373 | 1.00 | 36.24 |
| | ATOM | 3153 | CG1 | VAL | B | 458 | 9.827 | 10.650 | 13.324 | 1.00 | 38.50 |
| | ATOM | 3154 | CG2 | VAL | B | 458 | 9.463 | 12.699 | 14.701 | 1.00 | 39.84 |
| | ATOM | 3155 | C | VAL | B | 458 | 7.483 | 11.982 | 12.464 | 1.00 | 46.30 |
| | ATOM | 3156 | O | VAL | B | 458 | 7.567 | 13.201 | 12.302 | 1.00 | 47.67 |
| 40 | ATOM | 3157 | N | TYR | B | 459 | 7.393 | 11.138 | 11.442 | 1.00 | 50.45 |
| | ATOM | 3158 | CA | TYR | B | 459 | 7.385 | 11.640 | 10.069 | 1.00 | 57.07 |
| | ATOM | 3159 | CB | TYR | B | 459 | 8.233 | 10.740 | 9.170 | 1.00 | 57.05 |
| | ATOM | 3160 | CG | TYR | B | 459 | 9.673 | 10.680 | 9.611 | 1.00 | 59.29 |
| | ATOM | 3161 | CD1 | TYR | B | 459 | 10.284 | 11.786 | 10.203 | 1.00 | 60.93 |
| 45 | ATOM | 3162 | CE1 | TYR | B | 459 | 11.591 | 11.725 | 10.662 | 1.00 | 61.86 |
| | ATOM | 3163 | CD2 | TYR | B | 459 | 10.414 | 9.510 | 9.486 | 1.00 | 59.46 |
| | ATOM | 3164 | CE2 | TYR | B | 459 | 11.726 | 9.439 | 9.943 | 1.00 | 59.67 |
| | ATOM | 3165 | CZ | TYR | B | 459 | 12.305 | 10.548 | 10.532 | 1.00 | 60.84 |
| | ATOM | 3166 | OH | TYR | B | 459 | 13.593 | 10.477 | 11.009 | 1.00 | 61.39 |
| 50 | ATOM | 3167 | C | TYR | B | 459 | 5.976 | 11.753 | 9.514 | 1.00 | 61.22 |
| | ATOM | 3168 | O | TYR | B | 459 | 5.629 | 12.750 | 8.874 | 1.00 | 62.89 |
| | ATOM | 3169 | N | THR | B | 460 | 5.166 | 10.730 | 9.768 | 1.00 | 65.15 |
| | ATOM | 3170 | CA | THR | B | 460 | 3.783 | 10.702 | 9.309 | 1.00 | 67.76 |
| | ATOM | 3171 | CB | THR | B | 460 | 3.178 | 9.283 | 9.464 | 1.00 | 68.02 |
| 55 | ATOM | 3172 | OG1 | THR | B | 460 | 1.890 | 9.235 | 8.836 | 1.00 | 67.03 |
| | ATOM | 3173 | CG2 | THR | B | 460 | 3.040 | 8.916 | 10.938 | 1.00 | 67.31 |
| | ATOM | 3174 | C | THR | B | 460 | 2.945 | 11.700 | 10.107 | 1.00 | 70.14 |
| | ATOM | 3175 | O | THR | B | 460 | 1.715 | 11.641 | 10.099 | 1.00 | 72.35 |
| | ATOM | 3176 | N | PHE | B | 461 | 3.625 | 12.620 | 10.788 | 1.00 | 72.64 |
| 60 | ATOM | 3177 | CA | PHE | B | 461 | 2.969 | 13.637 | 11.607 | 1.00 | 75.05 |
| | ATOM | 3178 | CB | PHE | B | 461 | 3.977 | 14.720 | 12.012 | 1.00 | 75.47 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3179 | CG | PHE | B | 461 | 4.235 | 14.789 | 13.492 | 1.00 | 74.32 |
| | ATOM | 3180 | CD1 | PHE | B | 461 | 3.200 | 14.609 | 14.404 | 1.00 | 73.98 |
| | ATOM | 3181 | CD2 | PHE | B | 461 | 5.517 | 15.025 | 13.975 | 1.00 | 75.22 |
| | ATOM | 3182 | CE1 | PHE | B | 461 | 3.438 | 14.662 | 15.775 | 1.00 | 74.02 |
| | ATOM | 3183 | CE2 | PHE | B | 461 | 5.765 | 15.080 | 15.344 | 1.00 | 74.50 |
| 10 | ATOM | 3184 | CZ | PHE | B | 461 | 4.722 | 14.897 | 16.245 | 1.00 | 74.10 |
| | ATOM | 3185 | C | PHE | B | 461 | 1.787 | 14.286 | 10.896 | 1.00 | 76.78 |
| | ATOM | 3186 | O | PHE | B | 461 | 1.775 | 14.279 | 9.645 | 1.00 | 77.08 |
| | ATOM | 3187 | CB | GLU | B | 470 | 7.873 | 23.789 | 14.718 | 1.00 | 80.19 |
| | ATOM | 3188 | C | GLU | B | 470 | 8.958 | 21.731 | 15.650 | 1.00 | 79.30 |
| 15 | ATOM | 3189 | O | GLU | B | 470 | 9.887 | 21.518 | 16.432 | 1.00 | 78.21 |
| | ATOM | 3190 | N | GLU | B | 470 | 9.096 | 22.235 | 13.227 | 1.00 | 80.22 |
| | ATOM | 3191 | CA | GLU | B | 470 | 9.060 | 22.830 | 14.595 | 1.00 | 80.03 |
| | ATOM | 3192 | N | GLU | B | 471 | 7.823 | 21.037 | 15.665 | 1.00 | 78.31 |
| | ATOM | 3193 | CA | GLU | B | 471 | 7.596 | 19.956 | 16.617 | 1.00 | 75.83 |
| 20 | ATOM | 3194 | CB | GLU | B | 471 | 6.118 | 19.543 | 16.604 | 1.00 | 76.70 |
| | ATOM | 3195 | CG | GLU | B | 471 | 5.742 | 18.544 | 15.516 | 1.00 | 78.42 |
| | ATOM | 3196 | CD | GLU | B | 471 | 5.062 | 19.198 | 14.327 | 1.00 | 79.69 |
| | ATOM | 3197 | OE1 | GLU | B | 471 | 3.829 | 19.398 | 14.378 | 1.00 | 80.26 |
| | ATOM | 3198 | OE2 | GLU | B | 471 | 5.763 | 19.511 | 13.340 | 1.00 | 80.72 |
| 25 | ATOM | 3199 | C | GLU | B | 471 | 8.487 | 18.756 | 16.292 | 1.00 | 73.13 |
| | ATOM | 3200 | O | GLU | B | 471 | 8.897 | 18.021 | 17.189 | 1.00 | 73.86 |
| | ATOM | 3201 | N | LYS | B | 472 | 8.785 | 18.565 | 15.009 | 1.00 | 69.65 |
| | ATOM | 3202 | CA | LYS | B | 472 | 9.639 | 17.461 | 14.581 | 1.00 | 64.40 |
| | ATOM | 3203 | CB | LYS | B | 472 | 9.578 | 17.293 | 13.060 | 1.00 | 63.78 |
| 30 | ATOM | 3204 | CG | LYS | B | 472 | 8.343 | 16.552 | 12.566 | 1.00 | 64.49 |
| | ATOM | 3205 | CD | LYS | B | 472 | 8.544 | 16.002 | 11.161 | 1.00 | 63.81 |
| | ATOM | 3206 | CE | LYS | B | 472 | 7.379 | 16.368 | 10.249 | 1.00 | 64.90 |
| | ATOM | 3207 | NZ | LYS | B | 472 | 6.475 | 15.212 | 9.990 | 1.00 | 63.97 |
| | ATOM | 3208 | C | LYS | B | 472 | 11.071 | 17.749 | 15.014 | 1.00 | 61.03 |
| 35 | ATOM | 3209 | O | LYS | B | 472 | 11.848 | 16.833 | 15.287 | 1.00 | 60.28 |
| | ATOM | 3210 | N | ASP | B | 473 | 11.413 | 19.033 | 15.076 | 1.00 | 56.84 |
| | ATOM | 3211 | CA | ASP | B | 473 | 12.745 | 19.451 | 15.488 | 1.00 | 51.69 |
| | ATOM | 3212 | CB | ASP | B | 473 | 12.923 | 20.940 | 15.242 | 1.00 | 50.36 |
| | ATOM | 3213 | C | ASP | B | 473 | 12.923 | 19.138 | 16.970 | 1.00 | 49.18 |
| 40 | ATOM | 3214 | O | ASP | B | 473 | 13.959 | 18.619 | 17.385 | 1.00 | 46.85 |
| | ATOM | 3215 | N | HIS | B | 474 | 11.898 | 19.449 | 17.758 | 1.00 | 45.35 |
| | ATOM | 3216 | CA | HIS | B | 474 | 11.923 | 19.203 | 19.196 | 1.00 | 43.65 |
| | ATOM | 3217 | CB | HIS | B | 474 | 10.652 | 19.761 | 19.847 | 1.00 | 43.70 |
| | ATOM | 3218 | CG | HIS | B | 474 | 10.458 | 19.326 | 21.267 | 1.00 | 43.86 |
| 45 | ATOM | 3219 | CD2 | HIS | B | 474 | 11.095 | 19.688 | 22.406 | 1.00 | 44.12 |
| | ATOM | 3220 | ND1 | HIS | B | 474 | 9.510 | 18.395 | 21.638 | 1.00 | 46.60 |
| | ATOM | 3221 | CE1 | HIS | B | 474 | 9.572 | 18.202 | 22.943 | 1.00 | 45.29 |
| | ATOM | 3222 | NE2 | HIS | B | 474 | 10.526 | 18.975 | 23.434 | 1.00 | 47.96 |
| | ATOM | 3223 | C | HIS | B | 474 | 12.030 | 17.707 | 19.471 | 1.00 | 42.38 |
| 50 | ATOM | 3224 | O | HIS | B | 474 | 12.834 | 17.273 | 20.298 | 1.00 | 42.83 |
| | ATOM | 3225 | N | ILE | B | 475 | 11.214 | 16.923 | 18.773 | 1.00 | 38.86 |
| | ATOM | 3226 | CA | ILE | B | 475 | 11.222 | 15.475 | 18.943 | 1.00 | 36.53 |
| | ATOM | 3227 | CB | ILE | B | 475 | 10.105 | 14.822 | 18.110 | 1.00 | 36.56 |
| | ATOM | 3228 | CG2 | ILE | B | 475 | 10.390 | 13.335 | 17.911 | 1.00 | 36.17 |
| 55 | ATOM | 3229 | CG1 | ILE | B | 475 | 8.770 | 14.998 | 18.832 | 1.00 | 35.81 |
| | ATOM | 3230 | CD1 | ILE | B | 475 | 7.598 | 14.410 | 18.094 | 1.00 | 41.77 |
| | ATOM | 3231 | C | ILE | B | 475 | 12.575 | 14.898 | 18.532 | 1.00 | 33.72 |
| | ATOM | 3232 | O | ILE | B | 475 | 13.112 | 14.023 | 19.207 | 1.00 | 31.50 |
| | ATOM | 3233 | N | HIS | B | 476 | 13.121 | 15.375 | 17.429 | 1.00 | 33.65 |
| 60 | ATOM | 3234 | CA | HIS | B | 476 | 14.421 | 14.886 | 16.992 | 1.00 | 33.31 |
| | ATOM | 3235 | CB | HIS | B | 476 | 14.782 | 15.481 | 15.637 | 1.00 | 37.30 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3236 | CG | HIS | B | 476 | 14.132 | 14.781 | 14.486 | 1.00 | 43.64 |
| | ATOM | 3237 | CD2 | HIS | B | 476 | 13.723 | 13.498 | 14.342 | 1.00 | 45.25 |
| | ATOM | 3238 | ND1 | HIS | B | 476 | 13.816 | 15.419 | 13.306 | 1.00 | 48.37 |
| | ATOM | 3239 | CE1 | HIS | B | 476 | 13.238 | 14.560 | 12.484 | 1.00 | 48.87 |
| | ATOM | 3240 | NE2 | HIS | B | 476 | 13.170 | 13.387 | 13.089 | 1.00 | 48.11 |
| 10 | ATOM | 3241 | C | HIS | B | 476 | 15.506 | 15.213 | 18.022 | 1.00 | 31.20 |
| | ATOM | 3242 | O | HIS | B | 476 | 16.442 | 14.436 | 18.208 | 1.00 | 27.25 |
| | ATOM | 3243 | N | ARG | B | 477 | 15.387 | 16.365 | 18.684 | 1.00 | 30.64 |
| | ATOM | 3244 | CA | ARG | B | 477 | 16.361 | 16.754 | 19.703 | 1.00 | 30.09 |
| | ATOM | 3245 | CB | ARG | B | 477 | 16.144 | 18.214 | 20.121 | 1.00 | 33.46 |
| 15 | ATOM | 3246 | CG | ARG | B | 477 | 16.322 | 19.212 | 18.982 | 1.00 | 40.74 |
| | ATOM | 3247 | CD | ARG | B | 477 | 16.274 | 20.649 | 19.479 | 1.00 | 45.91 |
| | ATOM | 3248 | NE | ARG | B | 477 | 17.514 | 21.020 | 20.155 | 1.00 | 51.37 |
| | ATOM | 3249 | CZ | ARG | B | 477 | 18.375 | 21.927 | 19.702 | 1.00 | 53.68 |
| | ATOM | 3250 | NH1 | ARG | B | 477 | 18.140 | 22.567 | 18.560 | 1.00 | 53.04 |
| 20 | ATOM | 3251 | NH2 | ARG | B | 477 | 19.480 | 22.185 | 20.389 | 1.00 | 51.79 |
| | ATOM | 3252 | C | ARG | B | 477 | 16.232 | 15.835 | 20.925 | 1.00 | 26.97 |
| | ATOM | 3253 | O | ARG | B | 477 | 17.233 | 15.387 | 21.486 | 1.00 | 27.34 |
| | ATOM | 3254 | N | VAL | B | 478 | 14.999 | 15.558 | 21.338 | 1.00 | 23.70 |
| | ATOM | 3255 | CA | VAL | B | 478 | 14.780 | 14.685 | 22.482 | 1.00 | 24.79 |
| 25 | ATOM | 3256 | CB | VAL | B | 478 | 13.286 | 14.613 | 22.861 | 1.00 | 24.83 |
| | ATOM | 3257 | CG1 | VAL | B | 478 | 13.088 | 13.646 | 24.022 | 1.00 | 26.23 |
| | ATOM | 3258 | CG2 | VAL | B | 478 | 12.781 | 15.996 | 23.243 | 1.00 | 28.26 |
| | ATOM | 3259 | C | VAL | B | 478 | 15.284 | 13.294 | 22.112 | 1.00 | 26.10 |
| | ATOM | 3260 | O | VAL | B | 478 | 15.919 | 12.613 | 22.927 | 1.00 | 24.28 |
| 30 | ATOM | 3261 | N | LEU | B | 479 | 15.021 | 12.889 | 20.870 | 1.00 | 22.92 |
| | ATOM | 3262 | CA | LEU | B | 479 | 15.456 | 11.584 | 20.379 | 1.00 | 21.96 |
| | ATOM | 3263 | CB | LEU | B | 479 | 14.992 | 11.372 | 18.930 | 1.00 | 22.63 |
| | ATOM | 3264 | CG | LEU | B | 479 | 13.575 | 10.798 | 18.756 | 1.00 | 20.82 |
| | ATOM | 3265 | CD1 | LEU | B | 479 | 13.231 | 10.689 | 17.274 | 1.00 | 22.53 |
| 35 | ATOM | 3266 | CD2 | LEU | B | 479 | 13.495 | 9.440 | 19.420 | 1.00 | 23.08 |
| | ATOM | 3267 | C | LEU | B | 479 | 16.975 | 11.471 | 20.453 | 1.00 | 21.90 |
| | ATOM | 3268 | O | LEU | B | 479 | 17.506 | 10.416 | 20.778 | 1.00 | 23.11 |
| | ATOM | 3269 | N | ASP | B | 480 | 17.675 | 12.560 | 20.143 | 1.00 | 23.65 |
| | ATOM | 3270 | CA | ASP | B | 480 | 19.141 | 12.566 | 20.198 | 1.00 | 24.29 |
| 40 | ATOM | 3271 | CB | ASP | B | 480 | 19.692 | 13.889 | 19.649 | 1.00 | 26.88 |
| | ATOM | 3272 | CG | ASP | B | 480 | 19.773 | 13.914 | 18.129 | 1.00 | 33.32 |
| | ATOM | 3273 | OD1 | ASP | B | 480 | 19.857 | 12.836 | 17.499 | 1.00 | 35.44 |
| | ATOM | 3274 | OD2 | ASP | B | 480 | 19.757 | 15.022 | 17.563 | 1.00 | 32.44 |
| | ATOM | 3275 | C | ASP | B | 480 | 19.590 | 12.406 | 21.656 | 1.00 | 24.13 |
| 45 | ATOM | 3276 | O | ASP | B | 480 | 20.551 | 11.697 | 21.956 | 1.00 | 24.88 |
| | ATOM | 3277 | N | LYS | B | 481 | 18.887 | 13.077 | 22.560 | 1.00 | 25.18 |
| | ATOM | 3278 | CA | LYS | B | 481 | 19.213 | 13.010 | 23.980 | 1.00 | 26.78 |
| | ATOM | 3279 | CB | LYS | B | 481 | 18.262 | 13.898 | 24.785 | 1.00 | 31.37 |
| | ATOM | 3280 | CG | LYS | B | 481 | 18.962 | 14.788 | 25.804 | 1.00 | 43.84 |
| 50 | ATOM | 3281 | CD | LYS | B | 481 | 18.780 | 14.260 | 27.219 | 1.00 | 46.08 |
| | ATOM | 3282 | CE | LYS | B | 481 | 20.120 | 13.928 | 27.865 | 1.00 | 50.99 |
| | ATOM | 3283 | NZ | LYS | B | 481 | 21.177 | 14.922 | 27.511 | 1.00 | 54.35 |
| | ATOM | 3284 | C | LYS | B | 481 | 19.124 | 11.575 | 24.495 | 1.00 | 26.87 |
| | ATOM | 3285 | O | LYS | B | 481 | 19.951 | 11.145 | 25.305 | 1.00 | 20.37 |
| 55 | ATOM | 3286 | N | ILE | B | 482 | 18.124 | 10.830 | 24.027 | 1.00 | 23.26 |
| | ATOM | 3287 | CA | ILE | B | 482 | 17.981 | 9.452 | 24.472 | 1.00 | 21.07 |
| | ATOM | 3288 | CB | ILE | B | 482 | 16.655 | 8.828 | 24.015 | 1.00 | 19.80 |
| | ATOM | 3289 | CG2 | ILE | B | 482 | 16.580 | 7.370 | 24.491 | 1.00 | 17.40 |
| | ATOM | 3290 | CG1 | ILE | B | 482 | 15.479 | 9.606 | 24.602 | 1.00 | 17.16 |
| 60 | ATOM | 3291 | CD1 | ILE | B | 482 | 14.136 | 9.209 | 23.991 | 1.00 | 19.43 |
| | ATOM | 3292 | C | ILE | B | 482 | 19.135 | 8.616 | 23.947 | 1.00 | 20.21 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3293 | O | ILE | B | 482 | 19.621 | 7.722 | 24.640 | 1.00 | 25.55 |
| | ATOM | 3294 | N | THR | B | 483 | 19.569 | 8.896 | 22.722 | 1.00 | 21.89 |
| | ATOM | 3295 | CA | THR | B | 483 | 20.701 | 8.176 | 22.141 | 1.00 | 22.67 |
| | ATOM | 3296 | CB | THR | B | 483 | 21.030 | 8.662 | 20.695 | 1.00 | 23.34 |
| | ATOM | 3297 | OG1 | THR | B | 483 | 19.890 | 8.475 | 19.851 | 1.00 | 27.33 |
| 10 | ATOM | 3298 | CG2 | THR | B | 483 | 22.203 | 7.882 | 20.116 | 1.00 | 24.46 |
| | ATOM | 3299 | C | THR | B | 483 | 21.913 | 8.441 | 23.035 | 1.00 | 23.51 |
| | ATOM | 3300 | O | THR | B | 483 | 22.650 | 7.520 | 23.381 | 1.00 | 27.01 |
| | ATOM | 3301 | N | ASP | B | 484 | 22.119 | 9.703 | 23.404 | 1.00 | 22.88 |
| | ATOM | 3302 | CA | ASP | B | 484 | 23.237 | 10.058 | 24.276 | 1.00 | 24.93 |
| 15 | ATOM | 3303 | CB | ASP | B | 484 | 23.201 | 11.546 | 24.652 | 1.00 | 28.69 |
| | ATOM | 3304 | CG | ASP | B | 484 | 23.504 | 12.464 | 23.485 | 1.00 | 29.19 |
| | ATOM | 3305 | OD1 | ASP | B | 484 | 23.982 | 11.984 | 22.437 | 1.00 | 29.63 |
| | ATOM | 3306 | OD2 | ASP | B | 484 | 23.256 | 13.681 | 23.627 | 1.00 | 32.02 |
| | ATOM | 3307 | C | ASP | B | 484 | 23.125 | 9.249 | 25.567 | 1.00 | 24.40 |
| 20 | ATOM | 3308 | O | ASP | B | 484 | 24.125 | 8.780 | 26.103 | 1.00 | 25.60 |
| | ATOM | 3309 | N | THR | B | 485 | 21.899 | 9.096 | 26.066 | 1.00 | 20.16 |
| | ATOM | 3310 | CA | THR | B | 485 | 21.670 | 8.365 | 27.307 | 1.00 | 22.28 |
| | ATOM | 3311 | CB | THR | B | 485 | 20.203 | 8.521 | 27.763 | 1.00 | 24.64 |
| | ATOM | 3312 | OG1 | THR | B | 485 | 19.878 | 9.914 | 27.830 | 1.00 | 24.28 |
| 25 | ATOM | 3313 | CG2 | THR | B | 485 | 19.993 | 7.896 | 29.133 | 1.00 | 23.32 |
| | ATOM | 3314 | C | THR | B | 485 | 22.017 | 6.881 | 27.188 | 1.00 | 22.13 |
| | ATOM | 3315 | O | THR | B | 485 | 22.574 | 6.284 | 28.115 | 1.00 | 23.30 |
| | ATOM | 3316 | N | LEU | B | 486 | 21.686 | 6.290 | 26.045 | 1.00 | 23.08 |
| | ATOM | 3317 | CA | LEU | B | 486 | 21.969 | 4.881 | 25.792 | 1.00 | 22.26 |
| 30 | ATOM | 3318 | CB | LEU | B | 486 | 21.346 | 4.452 | 24.464 | 1.00 | 20.93 |
| | ATOM | 3319 | CG | LEU | B | 486 | 19.878 | 4.031 | 24.533 | 1.00 | 24.92 |
| | ATOM | 3320 | CD1 | LEU | B | 486 | 19.295 | 4.003 | 23.123 | 1.00 | 21.96 |
| | ATOM | 3321 | CD2 | LEU | B | 486 | 19.763 | 2.658 | 25.196 | 1.00 | 23.90 |
| | ATOM | 3322 | C | LEU | B | 486 | 23.477 | 4.634 | 25.742 | 1.00 | 24.12 |
| 35 | ATOM | 3323 | O | LEU | B | 486 | 23.984 | 3.681 | 26.334 | 1.00 | 24.02 |
| | ATOM | 3324 | N | ILE | B | 487 | 24.191 | 5.490 | 25.022 | 1.00 | 24.53 |
| | ATOM | 3325 | CA | ILE | B | 487 | 25.640 | 5.345 | 24.913 | 1.00 | 25.16 |
| | ATOM | 3326 | CB | ILE | B | 487 | 26.207 | 6.379 | 23.899 | 1.00 | 25.57 |
| | ATOM | 3327 | CG2 | ILE | B | 487 | 27.725 | 6.522 | 24.051 | 1.00 | 24.54 |
| 40 | ATOM | 3328 | CG1 | ILE | B | 487 | 25.857 | 5.936 | 22.470 | 1.00 | 25.63 |
| | ATOM | 3329 | CD1 | ILE | B | 487 | 26.538 | 4.646 | 22.021 | 1.00 | 25.68 |
| | ATOM | 3330 | C | ILE | B | 487 | 26.275 | 5.518 | 26.307 | 1.00 | 23.60 |
| | ATOM | 3331 | O | ILE | B | 487 | 27.200 | 4.794 | 26.671 | 1.00 | 23.65 |
| | ATOM | 3332 | N | HIS | B | 488 | 25.755 | 6.456 | 27.081 | 1.00 | 21.75 |
| 45 | ATOM | 3333 | CA | HIS | B | 488 | 26.251 | 6.720 | 28.431 | 1.00 | 26.07 |
| | ATOM | 3334 | CB | HIS | B | 488 | 25.450 | 7.871 | 29.041 | 1.00 | 26.99 |
| | ATOM | 3335 | CG | HIS | B | 488 | 25.818 | 8.196 | 30.455 | 1.00 | 33.06 |
| | ATOM | 3336 | CD2 | HIS | B | 488 | 25.245 | 7.838 | 31.629 | 1.00 | 32.79 |
| | ATOM | 3337 | ND1 | HIS | B | 488 | 26.869 | 9.025 | 30.779 | 1.00 | 36.45 |
| 50 | ATOM | 3338 | CE1 | HIS | B | 488 | 26.927 | 9.164 | 32.091 | 1.00 | 35.93 |
| | ATOM | 3339 | NE2 | HIS | B | 488 | 25.953 | 8.453 | 32.630 | 1.00 | 33.88 |
| | ATOM | 3340 | C | HIS | B | 488 | 26.123 | 5.463 | 29.292 | 1.00 | 26.85 |
| | ATOM | 3341 | O | HIS | B | 488 | 27.071 | 5.054 | 29.967 | 1.00 | 28.52 |
| | ATOM | 3342 | N | LEU | B | 489 | 24.949 | 4.850 | 29.266 | 1.00 | 28.00 |
| 55 | ATOM | 3343 | CA | LEU | B | 489 | 24.715 | 3.642 | 30.040 | 1.00 | 25.94 |
| | ATOM | 3344 | CB | LEU | B | 489 | 23.298 | 3.127 | 29.788 | 1.00 | 27.07 |
| | ATOM | 3345 | CG | LEU | B | 489 | 22.158 | 3.909 | 30.445 | 1.00 | 31.71 |
| | ATOM | 3346 | CD1 | LEU | B | 489 | 20.827 | 3.516 | 29.799 | 1.00 | 28.08 |
| | ATOM | 3347 | CD2 | LEU | B | 489 | 22.143 | 3.616 | 31.949 | 1.00 | 29.30 |
| 60 | ATOM | 3348 | C | LEU | B | 489 | 25.718 | 2.561 | 29.642 | 1.00 | 26.84 |
| | ATOM | 3349 | O | LEU | B | 489 | 26.241 | 1.832 | 30.486 | 1.00 | 20.86 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3350 | N | MET | B | 490 | 25.978 | 2.453 | 28.345 | 1.00 | 23.82 |
| | ATOM | 3351 | CA | MET | B | 490 | 26.900 | 1.438 | 27.857 | 1.00 | 26.38 |
| | ATOM | 3352 | CB | MET | B | 490 | 26.775 | 1.306 | 26.336 | 1.00 | 27.29 |
| | ATOM | 3353 | CG | MET | B | 490 | 25.418 | 0.776 | 25.895 | 1.00 | 21.68 |
| | ATOM | 3354 | SD | MET | B | 490 | 25.208 | 0.739 | 24.106 | 1.00 | 26.30 |
| 10 | ATOM | 3355 | CE | MET | B | 490 | 23.461 | 0.412 | 24.022 | 1.00 | 19.66 |
| | ATOM | 3356 | C | MET | B | 490 | 28.341 | 1.743 | 28.247 | 1.00 | 26.42 |
| | ATOM | 3357 | O | MET | B | 490 | 29.109 | 0.833 | 28.574 | 1.00 | 24.76 |
| | ATOM | 3358 | N | ALA | B | 491 | 28.713 | 3.018 | 28.207 | 1.00 | 26.67 |
| | ATOM | 3359 | CA | ALA | B | 491 | 30.074 | 3.394 | 28.577 | 1.00 | 30.73 |
| 15 | ATOM | 3360 | CB | ALA | B | 491 | 30.299 | 4.882 | 28.335 | 1.00 | 26.66 |
| | ATOM | 3361 | C | ALA | B | 491 | 30.250 | 3.053 | 30.056 | 1.00 | 32.08 |
| | ATOM | 3362 | O | ALA | B | 491 | 31.194 | 2.361 | 30.438 | 1.00 | 34.66 |
| | ATOM | 3363 | N | LYS | B | 492 | 29.316 | 3.523 | 30.878 | 1.00 | 33.17 |
| | ATOM | 3364 | CA | LYS | B | 492 | 29.354 | 3.267 | 32.309 | 1.00 | 32.82 |
| 20 | ATOM | 3365 | CB | LYS | B | 492 | 28.110 | 3.849 | 32.976 | 1.00 | 36.38 |
| | ATOM | 3366 | CG | LYS | B | 492 | 28.412 | 4.797 | 34.123 | 1.00 | 38.68 |
| | ATOM | 3367 | CD | LYS | B | 492 | 27.242 | 4.887 | 35.084 | 1.00 | 41.41 |
| | ATOM | 3368 | CE | LYS | B | 492 | 26.299 | 6.013 | 34.698 | 1.00 | 47.57 |
| | ATOM | 3369 | NZ | LYS | B | 492 | 26.395 | 7.184 | 35.618 | 1.00 | 50.76 |
| 25 | ATOM | 3370 | C | LYS | B | 492 | 29.453 | 1.771 | 32.619 | 1.00 | 34.08 |
| | ATOM | 3371 | O | LYS | B | 492 | 30.090 | 1.382 | 33.593 | 1.00 | 34.31 |
| | ATOM | 3372 | N | ALA | B | 493 | 28.835 | 0.935 | 31.788 | 1.00 | 32.03 |
| | ATOM | 3373 | CA | ALA | B | 493 | 28.867 | -0.510 | 31.998 | 1.00 | 30.70 |
| | ATOM | 3374 | CB | ALA | B | 493 | 27.719 | -1.181 | 31.245 | 1.00 | 28.80 |
| 30 | ATOM | 3375 | C | ALA | B | 493 | 30.201 | -1.156 | 31.606 | 1.00 | 33.75 |
| | ATOM | 3376 | O | ALA | B | 493 | 30.402 | -2.356 | 31.819 | 1.00 | 30.53 |
| | ATOM | 3377 | N | GLY | B | 494 | 31.102 | -0.372 | 31.020 | 1.00 | 33.50 |
| | ATOM | 3378 | CA | GLY | B | 494 | 32.405 | -0.903 | 30.656 | 1.00 | 33.71 |
| | ATOM | 3379 | C | GLY | B | 494 | 32.639 | -1.360 | 29.230 | 1.00 | 34.40 |
| 35 | ATOM | 3380 | O | GLY | B | 494 | 33.663 | -1.989 | 28.950 | 1.00 | 33.13 |
| | ATOM | 3381 | N | LEU | B | 495 | 31.712 | -1.056 | 28.326 | 1.00 | 31.76 |
| | ATOM | 3382 | CA | LEU | B | 495 | 31.859 | -1.452 | 26.925 | 1.00 | 30.57 |
| | ATOM | 3383 | CB | LEU | B | 495 | 30.494 | -1.415 | 26.216 | 1.00 | 30.67 |
| | ATOM | 3384 | CG | LEU | B | 495 | 29.610 | -2.675 | 26.256 | 1.00 | 29.59 |
| 40 | ATOM | 3385 | CD1 | LEU | B | 495 | 29.315 | -3.058 | 27.700 | 1.00 | 26.60 |
| | ATOM | 3386 | CD2 | LEU | B | 495 | 28.307 | -2.416 | 25.501 | 1.00 | 27.52 |
| | ATOM | 3387 | C | LEU | B | 495 | 32.829 | -0.515 | 26.202 | 1.00 | 30.53 |
| | ATOM | 3388 | O | LEU | B | 495 | 32.855 | 0.688 | 26.468 | 1.00 | 28.14 |
| | ATOM | 3389 | N | THR | B | 496 | 33.628 | -1.064 | 25.291 | 1.00 | 28.03 |
| 45 | ATOM | 3390 | CA | THR | B | 496 | 34.567 | -0.243 | 24.529 | 1.00 | 29.06 |
| | ATOM | 3391 | CB | THR | B | 496 | 35.511 | -1.095 | 23.665 | 1.00 | 29.40 |
| | ATOM | 3392 | OG1 | THR | B | 496 | 34.753 | -1.758 | 22.641 | 1.00 | 30.29 |
| | ATOM | 3393 | CG2 | THR | B | 496 | 36.228 | -2.122 | 24.515 | 1.00 | 28.12 |
| | ATOM | 3394 | C | THR | B | 496 | 33.770 | 0.652 | 23.590 | 1.00 | 30.12 |
| 50 | ATOM | 3395 | O | THR | B | 496 | 32.580 | 0.433 | 23.380 | 1.00 | 29.74 |
| | ATOM | 3396 | N | LEU | B | 497 | 34.430 | 1.654 | 23.018 | 1.00 | 30.44 |
| | ATOM | 3397 | CA | LEU | B | 497 | 33.762 | 2.567 | 22.104 | 1.00 | 28.54 |
| | ATOM | 3398 | CB | LEU | B | 497 | 34.768 | 3.564 | 21.529 | 1.00 | 31.14 |
| | ATOM | 3399 | CG | LEU | B | 497 | 35.209 | 4.719 | 22.434 | 1.00 | 33.58 |
| 55 | ATOM | 3400 | CD1 | LEU | B | 497 | 36.120 | 5.659 | 21.652 | 1.00 | 31.42 |
| | ATOM | 3401 | CD2 | LEU | B | 497 | 33.992 | 5.469 | 22.942 | 1.00 | 35.08 |
| | ATOM | 3402 | C | LEU | B | 497 | 33.095 | 1.800 | 20.967 | 1.00 | 27.35 |
| | ATOM | 3403 | O | LEU | B | 497 | 31.967 | 2.105 | 20.574 | 1.00 | 24.03 |
| | ATOM | 3404 | N | GLN | B | 498 | 33.798 | 0.797 | 20.447 | 1.00 | 26.17 |
| 60 | ATOM | 3405 | CA | GLN | B | 498 | 33.289 | -0.009 | 19.348 | 1.00 | 26.32 |
| | ATOM | 3406 | CB | GLN | B | 498 | 34.411 | -0.876 | 18.771 | 1.00 | 27.25 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3407 | CG | GLN | B | 498 | 33.967 | -1.796 | 17.645 | 1.00 | 32.67 |
| | ATOM | 3408 | CD | GLN | B | 498 | 34.965 | -2.912 | 17.374 | 1.00 | 38.39 |
| | ATOM | 3409 | OE1 | GLN | B | 498 | 35.737 | -3.298 | 18.254 | 1.00 | 36.78 |
| | ATOM | 3410 | NE2 | GLN | B | 498 | 34.953 | -3.437 | 16.153 | 1.00 | 33.18 |
| | ATOM | 3411 | C | GLN | B | 498 | 32.112 | -0.888 | 19.774 | 1.00 | 25.70 |
| 10 | ATOM | 3412 | O | GLN | B | 498 | 31.167 | -1.076 | 19.009 | 1.00 | 25.35 |
| | ATOM | 3413 | N | GLN | B | 499 | 32.173 | -1.434 | 20.986 | 1.00 | 24.01 |
| | ATOM | 3414 | CA | GLN | B | 499 | 31.093 | -2.281 | 21.487 | 1.00 | 25.34 |
| | ATOM | 3415 | CB | GLN | B | 499 | 31.501 | -2.935 | 22.815 | 1.00 | 28.38 |
| | ATOM | 3416 | CG | GLN | B | 499 | 32.537 | -4.056 | 22.669 | 1.00 | 29.13 |
| 15 | ATOM | 3417 | CD | GLN | B | 499 | 32.913 | -4.687 | 23.995 | 1.00 | 30.80 |
| | ATOM | 3418 | OE1 | GLN | B | 499 | 33.306 | -3.997 | 24.937 | 1.00 | 33.62 |
| | ATOM | 3419 | NE2 | GLN | B | 499 | 32.797 | -6.004 | 24.074 | 1.00 | 30.64 |
| | ATOM | 3420 | C | GLN | B | 499 | 29.842 | -1.430 | 21.693 | 1.00 | 25.70 |
| | ATOM | 3421 | O | GLN | B | 499 | 28.715 | -1.910 | 21.554 | 1.00 | 26.22 |
| 20 | ATOM | 3422 | N | GLN | B | 500 | 30.062 | -0.160 | 22.020 | 1.00 | 23.09 |
| | ATOM | 3423 | CA | GLN | B | 500 | 28.989 | 0.793 | 22.256 | 1.00 | 23.53 |
| | ATOM | 3424 | CB | GLN | B | 500 | 29.564 | 2.107 | 22.782 | 1.00 | 26.17 |
| | ATOM | 3425 | CG | GLN | B | 500 | 29.958 | 2.073 | 24.252 | 1.00 | 27.71 |
| | ATOM | 3426 | CD | GLN | B | 500 | 30.812 | 3.262 | 24.641 | 1.00 | 29.32 |
| 25 | ATOM | 3427 | OE1 | GLN | B | 500 | 30.559 | 4.386 | 24.207 | 1.00 | 28.48 |
| | ATOM | 3428 | NE2 | GLN | B | 500 | 31.831 | 3.021 | 25.463 | 1.00 | 25.07 |
| | ATOM | 3429 | C | GLN | B | 500 | 28.151 | 1.074 | 21.015 | 1.00 | 24.24 |
| | ATOM | 3430 | O | GLN | B | 500 | 26.923 | 0.949 | 21.053 | 1.00 | 24.40 |
| | ATOM | 3431 | N | HIS | B | 501 | 28.790 | 1.465 | 19.915 | 1.00 | 23.08 |
| 30 | ATOM | 3432 | CA | HIS | B | 501 | 28.004 | 1.739 | 18.724 | 1.00 | 26.92 |
| | ATOM | 3433 | CB | HIS | B | 501 | 28.791 | 2.577 | 17.697 | 1.00 | 32.00 |
| | ATOM | 3434 | CG | HIS | B | 501 | 29.988 | 1.896 | 17.105 | 1.00 | 36.97 |
| | ATOM | 3435 | CD2 | HIS | B | 501 | 30.122 | 0.710 | 16.465 | 1.00 | 40.32 |
| | ATOM | 3436 | ND1 | HIS | B | 501 | 31.224 | 2.505 | 17.042 | 1.00 | 37.88 |
| 35 | ATOM | 3437 | CE1 | HIS | B | 501 | 32.066 | 1.724 | 16.389 | 1.00 | 38.81 |
| | ATOM | 3438 | NE2 | HIS | B | 501 | 31.422 | 0.628 | 16.028 | 1.00 | 41.21 |
| | ATOM | 3439 | C | HIS | B | 501 | 27.451 | 0.457 | 18.123 | 1.00 | 25.91 |
| | ATOM | 3440 | O | HIS | B | 501 | 26.369 | 0.457 | 17.531 | 1.00 | 20.13 |
| | ATOM | 3441 | N | GLN | B | 502 | 28.165 | -0.648 | 18.317 | 1.00 | 24.94 |
| 40 | ATOM | 3442 | CA | GLN | B | 502 | 27.698 | -1.926 | 17.804 | 1.00 | 21.88 |
| | ATOM | 3443 | CB | GLN | B | 502 | 28.785 | -2.996 | 17.953 | 1.00 | 24.62 |
| | ATOM | 3444 | CG | GLN | B | 502 | 29.796 | -3.001 | 16.797 | 1.00 | 26.55 |
| | ATOM | 3445 | CD | GLN | B | 502 | 30.843 | -4.109 | 16.902 | 1.00 | 27.06 |
| | ATOM | 3446 | OE1 | GLN | B | 502 | 30.716 | -5.033 | 17.705 | 1.00 | 28.49 |
| 45 | ATOM | 3447 | NE2 | GLN | B | 502 | 31.882 | -4.018 | 16.078 | 1.00 | 21.90 |
| | ATOM | 3448 | C | GLN | B | 502 | 26.428 | -2.341 | 18.554 | 1.00 | 22.39 |
| | ATOM | 3449 | O | GLN | B | 502 | 25.464 | -2.807 | 17.944 | 1.00 | 22.24 |
| | ATOM | 3450 | N | ARG | B | 503 | 26.421 | -2.159 | 19.874 | 1.00 | 20.54 |
| | ATOM | 3451 | CA | ARG | B | 503 | 25.259 | -2.523 | 20.678 | 1.00 | 22.04 |
| 50 | ATOM | 3452 | CB | ARG | B | 503 | 25.602 | -2.519 | 22.180 | 1.00 | 22.51 |
| | ATOM | 3453 | CG | ARG | B | 503 | 24.451 | -3.022 | 23.077 | 1.00 | 23.34 |
| | ATOM | 3454 | CD | ARG | B | 503 | 24.853 | -3.110 | 24.550 | 1.00 | 22.18 |
| | ATOM | 3455 | NE | ARG | B | 503 | 23.743 | -3.546 | 25.395 | 1.00 | 19.62 |
| | ATOM | 3456 | CZ | ARG | B | 503 | 23.329 | -4.807 | 25.497 | 1.00 | 19.88 |
| 55 | ATOM | 3457 | NH1 | ARG | B | 503 | 23.933 | -5.765 | 24.809 | 1.00 | 16.40 |
| | ATOM | 3458 | NH2 | ARG | B | 503 | 22.303 | -5.110 | 26.280 | 1.00 | 19.71 |
| | ATOM | 3459 | C | ARG | B | 503 | 24.102 | -1.558 | 20.409 | 1.00 | 19.05 |
| | ATOM | 3460 | O | ARG | B | 503 | 22.945 | -1.968 | 20.351 | 1.00 | 18.87 |
| | ATOM | 3461 | N | LEU | B | 504 | 24.414 | -0.276 | 20.239 | 1.00 | 20.19 |
| 60 | ATOM | 3462 | CA | LEU | B | 504 | 23.375 | 0.714 | 19.969 | 1.00 | 19.33 |
| | ATOM | 3463 | CB | LEU | B | 504 | 23.972 | 2.117 | 19.855 | 1.00 | 16.25 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3464 | CG | LEU | B | 504 | 22.983 | 3.173 | 19.344 | 1.00 | 20.35 |
| | ATOM | 3465 | CD1 | LEU | B | 504 | 21.930 | 3.449 | 20.427 | 1.00 | 17.97 |
| | ATOM | 3466 | CD2 | LEU | B | 504 | 23.729 | 4.448 | 18.955 | 1.00 | 20.86 |
| | ATOM | 3467 | C | LEU | B | 504 | 22.659 | 0.357 | 18.667 | 1.00 | 21.22 |
| | ATOM | 3468 | O | LEU | B | 504 | 21.433 | 0.478 | 18.566 | 1.00 | 19.28 |
| 10 | ATOM | 3469 | N | ALA | B | 505 | 23.428 | -0.085 | 17.676 | 1.00 | 18.55 |
| | ATOM | 3470 | CA | ALA | B | 505 | 22.859 | -0.473 | 16.396 | 1.00 | 18.20 |
| | ATOM | 3471 | CB | ALA | B | 505 | 23.973 | -0.745 | 15.382 | 1.00 | 18.45 |
| | ATOM | 3472 | C | ALA | B | 505 | 21.986 | -1.716 | 16.562 | 1.00 | 19.54 |
| | ATOM | 3473 | O | ALA | B | 505 | 20.871 | -1.774 | 16.041 | 1.00 | 17.63 |
| 15 | ATOM | 3474 | N | GLN | B | 506 | 22.497 | -2.706 | 17.293 | 1.00 | 20.30 |
| | ATOM | 3475 | CA | GLN | B | 506 | 21.772 | -3.955 | 17.513 | 1.00 | 19.48 |
| | ATOM | 3476 | CB | GLN | B | 506 | 22.590 | -4.893 | 18.409 | 1.00 | 21.75 |
| | ATOM | 3477 | CG | GLN | B | 506 | 23.798 | -5.551 | 17.727 | 1.00 | 20.85 |
| | ATOM | 3478 | CD | GLN | B | 506 | 24.819 | -6.070 | 18.736 | 1.00 | 26.18 |
| 20 | ATOM | 3479 | OE1 | GLN | B | 506 | 24.564 | -6.084 | 19.943 | 1.00 | 21.83 |
| | ATOM | 3480 | NE2 | GLN | B | 506 | 25.977 | -6.499 | 18.245 | 1.00 | 25.39 |
| | ATOM | 3481 | C | GLN | B | 506 | 20.421 | -3.672 | 18.166 | 1.00 | 21.39 |
| | ATOM | 3482 | O | GLN | B | 506 | 19.396 | -4.233 | 17.766 | 1.00 | 20.87 |
| | ATOM | 3483 | N | LEU | B | 507 | 20.433 | -2.800 | 19.171 | 1.00 | 19.52 |
| 25 | ATOM | 3484 | CA | LEU | B | 507 | 19.219 | -2.418 | 19.884 | 1.00 | 23.04 |
| | ATOM | 3485 | CB | LEU | B | 507 | 19.548 | -1.455 | 21.030 | 1.00 | 22.82 |
| | ATOM | 3486 | CG | LEU | B | 507 | 20.182 | -2.011 | 22.313 | 1.00 | 26.12 |
| | ATOM | 3487 | CD1 | LEU | B | 507 | 20.203 | -0.916 | 23.360 | 1.00 | 29.33 |
| | ATOM | 3488 | CD2 | LEU | B | 507 | 19.415 | -3.213 | 22.816 | 1.00 | 27.80 |
| 30 | ATOM | 3489 | C | LEU | B | 507 | 18.212 | -1.730 | 18.971 | 1.00 | 22.19 |
| | ATOM | 3490 | O | LEU | B | 507 | 17.036 | -2.070 | 18.964 | 1.00 | 23.00 |
| | ATOM | 3491 | N | LEU | B | 508 | 18.678 | -0.745 | 18.214 | 1.00 | 21.53 |
| | ATOM | 3492 | CA | LEU | B | 508 | 17.797 | 0.006 | 17.332 | 1.00 | 20.60 |
| | ATOM | 3493 | CB | LEU | B | 508 | 18.535 | 1.236 | 16.805 | 1.00 | 17.57 |
| 35 | ATOM | 3494 | CG | LEU | B | 508 | 18.934 | 2.218 | 17.913 | 1.00 | 17.67 |
| | ATOM | 3495 | CD1 | LEU | B | 508 | 19.566 | 3.446 | 17.301 | 1.00 | 20.04 |
| | ATOM | 3496 | CD2 | LEU | B | 508 | 17.724 | 2.611 | 18.725 | 1.00 | 18.49 |
| | ATOM | 3497 | C | LEU | B | 508 | 17.235 | -0.831 | 16.183 | 1.00 | 21.17 |
| | ATOM | 3498 | O | LEU | B | 508 | 16.118 | -0.597 | 15.728 | 1.00 | 21.88 |
| 40 | ATOM | 3499 | N | LEU | B | 509 | 18.000 | -1.813 | 15.713 | 1.00 | 21.89 |
| | ATOM | 3500 | CA | LEU | B | 509 | 17.511 | -2.657 | 14.631 | 1.00 | 22.81 |
| | ATOM | 3501 | CB | LEU | B | 509 | 18.603 | -3.597 | 14.145 | 1.00 | 22.65 |
| | ATOM | 3502 | CG | LEU | B | 509 | 19.645 | -2.891 | 13.278 | 1.00 | 29.11 |
| | ATOM | 3503 | CD1 | LEU | B | 509 | 20.697 | -3.888 | 12.829 | 1.00 | 25.69 |
| 45 | ATOM | 3504 | CD2 | LEU | B | 509 | 18.965 | -2.248 | 12.082 | 1.00 | 27.92 |
| | ATOM | 3505 | C | LEU | B | 509 | 16.302 | -3.462 | 15.095 | 1.00 | 23.32 |
| | ATOM | 3506 | O | LEU | B | 509 | 15.409 | -3.759 | 14.303 | 1.00 | 23.36 |
| | ATOM | 3507 | N | ILE | B | 510 | 16.264 | -3.796 | 16.380 | 1.00 | 23.36 |
| | ATOM | 3508 | CA | ILE | B | 510 | 15.148 | -4.562 | 16.912 | 1.00 | 20.99 |
| 50 | ATOM | 3509 | CB | ILE | B | 510 | 15.448 | -5.041 | 18.361 | 1.00 | 28.60 |
| | ATOM | 3510 | CG2 | ILE | B | 510 | 14.162 | -5.435 | 19.075 | 1.00 | 28.10 |
| | ATOM | 3511 | CG1 | ILE | B | 510 | 16.383 | -6.260 | 18.308 | 1.00 | 26.57 |
| | ATOM | 3512 | CD1 | ILE | B | 510 | 17.429 | -6.301 | 19.419 | 1.00 | 30.14 |
| | ATOM | 3513 | C | ILE | B | 510 | 13.852 | -3.746 | 16.846 | 1.00 | 17.65 |
| 55 | ATOM | 3514 | O | ILE | B | 510 | 12.767 | -4.308 | 16.759 | 1.00 | 16.11 |
| | ATOM | 3515 | N | LEU | B | 511 | 13.961 | -2.421 | 16.867 | 1.00 | 18.12 |
| | ATOM | 3516 | CA | LEU | B | 511 | 12.772 | -1.574 | 16.774 | 1.00 | 16.95 |
| | ATOM | 3517 | CB | LEU | B | 511 | 13.147 | -0.100 | 16.981 | 1.00 | 22.66 |
| | ATOM | 3518 | CG | LEU | B | 511 | 13.607 | 0.262 | 18.406 | 1.00 | 22.13 |
| 60 | ATOM | 3519 | CD1 | LEU | B | 511 | 13.404 | 1.751 | 18.652 | 1.00 | 25.29 |
| | ATOM | 3520 | CD2 | LEU | B | 511 | 12.830 | -0.549 | 19.425 | 1.00 | 25.08 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3521 | C | LEU | B | 511 | 12.112 | -1.771 | 15.397 | 1.00 | 16.65 |
| | ATOM | 3522 | O | LEU | B | 511 | 10.915 | -1.578 | 15.242 | 1.00 | 17.09 |
| | ATOM | 3523 | N | SER | B | 512 | 12.901 | -2.161 | 14.401 | 1.00 | 15.83 |
| | ATOM | 3524 | CA | SER | B | 512 | 12.355 | -2.408 | 13.072 | 1.00 | 18.66 |
| | ATOM | 3525 | CB | SER | B | 512 | 13.484 | -2.644 | 12.074 | 1.00 | 17.62 |
| 10 | ATOM | 3526 | OG | SER | B | 512 | 13.079 | -3.550 | 11.062 | 1.00 | 32.77 |
| | ATOM | 3527 | C | SER | B | 512 | 11.454 | -3.638 | 13.154 | 1.00 | 18.54 |
| | ATOM | 3528 | O | SER | B | 512 | 10.373 | -3.683 | 12.545 | 1.00 | 17.01 |
| | ATOM | 3529 | N | HIS | B | 513 | 11.899 | -4.625 | 13.929 | 1.00 | 15.54 |
| | ATOM | 3530 | CA | HIS | B | 513 | 11.141 | -5.860 | 14.115 | 1.00 | 17.67 |
| 15 | ATOM | 3531 | CB | HIS | B | 513 | 12.013 | -6.916 | 14.790 | 1.00 | 19.03 |
| | ATOM | 3532 | CG | HIS | B | 513 | 13.063 | -7.475 | 13.886 | 1.00 | 27.06 |
| | ATOM | 3533 | CD2 | HIS | B | 513 | 12.980 | -8.364 | 12.868 | 1.00 | 28.40 |
| | ATOM | 3534 | ND1 | HIS | B | 513 | 14.378 | -7.066 | 13.932 | 1.00 | 28.92 |
| | ATOM | 3535 | CE1 | HIS | B | 513 | 15.061 | -7.678 | 12.981 | 1.00 | 30.75 |
| 20 | ATOM | 3536 | NE2 | HIS | B | 513 | 14.235 | -8.472 | 12.321 | 1.00 | 30.08 |
| | ATOM | 3537 | C | HIS | B | 513 | 9.895 | -5.602 | 14.958 | 1.00 | 15.35 |
| | ATOM | 3538 | O | HIS | B | 513 | 8.846 | -6.192 | 14.704 | 1.00 | 14.83 |
| | ATOM | 3539 | N | ILE | B | 514 | 10.012 | -4.744 | 15.942 | 1.00 | 13.35 |
| | ATOM | 3540 | CA | ILE | B | 514 | 8.865 | -4.417 | 16.776 | 1.00 | 15.48 |
| 25 | ATOM | 3541 | CB | ILE | B | 514 | 9.295 | -3.534 | 17.967 | 1.00 | 20.02 |
| | ATOM | 3542 | CG2 | ILE | B | 514 | 8.067 | -2.918 | 18.650 | 1.00 | 12.84 |
| | ATOM | 3543 | CG1 | ILE | B | 514 | 10.093 | -4.397 | 18.962 | 1.00 | 22.87 |
| | ATOM | 3544 | CD1 | ILE | B | 514 | 10.691 | -3.641 | 20.115 | 1.00 | 29.62 |
| | ATOM | 3545 | C | ILE | B | 514 | 7.797 | -3.717 | 15.923 | 1.00 | 15.16 |
| 30 | ATOM | 3546 | O | ILE | B | 514 | 6.606 | -3.972 | 16.078 | 1.00 | 16.61 |
| | ATOM | 3547 | N | ARG | B | 515 | 8.224 | -2.823 | 15.030 | 1.00 | 16.33 |
| | ATOM | 3548 | CA | ARG | B | 515 | 7.280 | -2.138 | 14.150 | 1.00 | 17.54 |
| | ATOM | 3549 | CB | ARG | B | 515 | 8.010 | -1.173 | 13.214 | 1.00 | 20.15 |
| | ATOM | 3550 | CG | ARG | B | 515 | 7.080 | -0.454 | 12.234 | 1.00 | 21.47 |
| 35 | ATOM | 3551 | CD | ARG | B | 515 | 6.407 | 0.749 | 12.891 | 1.00 | 26.05 |
| | ATOM | 3552 | NE | ARG | B | 515 | 7.220 | 1.948 | 12.716 | 1.00 | 24.91 |
| | ATOM | 3553 | CZ | ARG | B | 515 | 6.734 | 3.175 | 12.547 | 1.00 | 24.61 |
| | ATOM | 3554 | NH1 | ARG | B | 515 | 5.424 | 3.393 | 12.522 | 1.00 | 22.46 |
| | ATOM | 3555 | NH2 | ARG | B | 515 | 7.569 | 4.182 | 12.374 | 1.00 | 23.15 |
| 40 | ATOM | 3556 | C | ARG | B | 515 | 6.545 | -3.182 | 13.304 | 1.00 | 16.60 |
| | ATOM | 3557 | O | ARG | B | 515 | 5.332 | -3.093 | 13.087 | 1.00 | 14.51 |
| | ATOM | 3558 | N | HIS | B | 516 | 7.298 | -4.171 | 12.827 | 1.00 | 18.50 |
| | ATOM | 3559 | CA | HIS | B | 516 | 6.743 | -5.237 | 11.997 | 1.00 | 17.26 |
| | ATOM | 3560 | CB | HIS | B | 516 | 7.861 | -6.176 | 11.533 | 1.00 | 18.14 |
| 45 | ATOM | 3561 | CG | HIS | B | 516 | 7.405 | -7.223 | 10.568 | 1.00 | 24.87 |
| | ATOM | 3562 | CD2 | HIS | B | 516 | 7.060 | -8.521 | 10.754 | 1.00 | 26.64 |
| | ATOM | 3563 | ND1 | HIS | B | 516 | 7.258 | -6.978 | 9.220 | 1.00 | 21.82 |
| | ATOM | 3564 | CE1 | HIS | B | 516 | 6.839 | -8.078 | 8.619 | 1.00 | 28.42 |
| | ATOM | 3565 | NE2 | HIS | B | 516 | 6.711 | -9.028 | 9.526 | 1.00 | 24.47 |
| 50 | ATOM | 3566 | C | HIS | B | 516 | 5.685 | -6.028 | 12.759 | 1.00 | 16.87 |
| | ATOM | 3567 | O | HIS | B | 516 | 4.596 | -6.303 | 12.240 | 1.00 | 14.81 |
| | ATOM | 3568 | N | MET | B | 517 | 5.999 | -6.396 | 13.997 | 1.00 | 16.48 |
| | ATOM | 3569 | CA | MET | B | 517 | 5.049 | -7.162 | 14.801 | 1.00 | 15.39 |
| | ATOM | 3570 | CB | MET | B | 517 | 5.701 | -7.587 | 16.114 | 1.00 | 21.05 |
| 55 | ATOM | 3571 | CG | MET | B | 517 | 6.790 | -8.638 | 15.917 | 1.00 | 20.76 |
| | ATOM | 3572 | SD | MET | B | 517 | 7.380 | -9.320 | 17.470 | 1.00 | 23.96 |
| | ATOM | 3573 | CE | MET | B | 517 | 8.104 | -7.879 | 18.226 | 1.00 | 20.45 |
| | ATOM | 3574 | C | MET | B | 517 | 3.789 | -6.368 | 15.080 | 1.00 | 16.23 |
| | ATOM | 3575 | O | MET | B | 517 | 2.688 | -6.924 | 15.148 | 1.00 | 16.02 |
| 60 | ATOM | 3576 | N | SER | B | 518 | 3.954 | -5.060 | 15.247 | 1.00 | 13.32 |
| | ATOM | 3577 | CA | SER | B | 518 | 2.827 | -4.186 | 15.505 | 1.00 | 16.34 |

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 3578 | CB | SER | B | 518 | 3.316 | -2.765 | 15.835 | 1.00 | 17.48 |
| | ATOM | 3579 | OG | SER | B | 518 | 2.234 | -1.840 | 15.843 | 1.00 | 17.46 |
| | ATOM | 3580 | C | SER | B | 518 | 1.906 | -4.147 | 14.284 | 1.00 | 14.73 |
| | ATOM | 3581 | O | SER | B | 518 | 0.688 | -4.247 | 14.417 | 1.00 | 19.16 |
| | ATOM | 3582 | N | ASN | B | 519 | 2.474 | -4.006 | 13.091 | 1.00 | 14.52 |
| 10 | ATOM | 3583 | CA | ASN | B | 519 | 1.622 | -3.953 | 11.907 | 1.00 | 15.35 |
| | ATOM | 3584 | CB | ASN | B | 519 | 2.432 | -3.509 | 10.698 | 1.00 | 19.21 |
| | ATOM | 3585 | CG | ASN | B | 519 | 2.700 | -2.029 | 10.729 | 1.00 | 20.58 |
| | ATOM | 3586 | OD1 | ASN | B | 519 | 1.839 | -1.258 | 11.150 | 1.00 | 26.36 |
| | ATOM | 3587 | ND2 | ASN | B | 519 | 3.891 | -1.618 | 10.307 | 1.00 | 19.62 |
| 15 | ATOM | 3588 | C | ASN | B | 519 | 0.911 | -5.280 | 11.658 | 1.00 | 16.74 |
| | ATOM | 3589 | O | ASN | B | 519 | -0.265 | -5.299 | 11.297 | 1.00 | 20.58 |
| | ATOM | 3590 | N | LYS | B | 520 | 1.608 | -6.387 | 11.885 | 1.00 | 18.60 |
| | ATOM | 3591 | CA | LYS | B | 520 | 0.992 | -7.699 | 11.717 | 1.00 | 20.04 |
| | ATOM | 3592 | CB | LYS | B | 520 | 2.038 | -8.801 | 11.872 | 1.00 | 25.44 |
| 20 | ATOM | 3593 | CG | LYS | B | 520 | 3.037 | -8.849 | 10.728 | 1.00 | 31.68 |
| | ATOM | 3594 | CD | LYS | B | 520 | 2.507 | -9.663 | 9.558 | 1.00 | 42.56 |
| | ATOM | 3595 | CE | LYS | B | 520 | 2.186 | -8.778 | 8.364 | 1.00 | 45.61 |
| | ATOM | 3596 | NZ | LYS | B | 520 | 1.435 | -9.526 | 7.312 | 1.00 | 46.00 |
| | ATOM | 3597 | C | LYS | B | 520 | -0.099 | -7.868 | 12.769 | 1.00 | 18.88 |
| 25 | ATOM | 3598 | O | LYS | B | 520 | -1.183 | -8.358 | 12.478 | 1.00 | 21.75 |
| | ATOM | 3599 | N | GLY | B | 521 | 0.191 | -7.455 | 13.998 | 1.00 | 17.83 |
| | ATOM | 3600 | CA | GLY | B | 521 | -0.792 | -7.569 | 15.058 | 1.00 | 16.19 |
| | ATOM | 3601 | C | GLY | B | 521 | -2.000 | -6.674 | 14.833 | 1.00 | 16.59 |
| | ATOM | 3602 | O | GLY | B | 521 | -3.128 | -7.060 | 15.125 | 1.00 | 16.57 |
| 30 | ATOM | 3603 | N | MET | B | 522 | -1.766 | -5.467 | 14.326 | 1.00 | 17.48 |
| | ATOM | 3604 | CA | MET | B | 522 | -2.852 | -4.527 | 14.042 | 1.00 | 18.25 |
| | ATOM | 3605 | CB | MET | B | 522 | -2.276 | -3.212 | 13.516 | 1.00 | 21.27 |
| | ATOM | 3606 | CG | MET | B | 522 | -3.190 | -2.018 | 13.707 | 1.00 | 26.97 |
| | ATOM | 3607 | SD | MET | B | 522 | -3.199 | -1.477 | 15.417 | 1.00 | 30.35 |
| 35 | ATOM | 3608 | CE | MET | B | 522 | -1.659 | -0.605 | 15.475 | 1.00 | 29.86 |
| | ATOM | 3609 | C | MET | B | 522 | -3.794 | -5.119 | 12.989 | 1.00 | 18.68 |
| | ATOM | 3610 | O | MET | B | 522 | -5.022 | -5.008 | 13.097 | 1.00 | 18.80 |
| | ATOM | 3611 | N | GLU | B | 523 | -3.205 | -5.731 | 11.966 | 1.00 | 18.22 |
| | ATOM | 3612 | CA | GLU | B | 523 | -3.968 | -6.357 | 10.889 | 1.00 | 23.41 |
| 40 | ATOM | 3613 | CB | GLU | B | 523 | -3.031 | -6.946 | 9.830 | 1.00 | 28.74 |
| | ATOM | 3614 | CG | GLU | B | 523 | -2.224 | -5.935 | 9.030 | 1.00 | 34.42 |
| | ATOM | 3615 | CD | GLU | B | 523 | -1.095 | -6.597 | 8.239 | 1.00 | 45.58 |
| | ATOM | 3616 | OE1 | GLU | B | 523 | -0.131 | -5.894 | 7.857 | 1.00 | 49.48 |
| | ATOM | 3617 | OE2 | GLU | B | 523 | -1.169 | -7.825 | 7.999 | 1.00 | 45.97 |
| 45 | ATOM | 3618 | C | GLU | B | 523 | -4.812 | -7.482 | 11.465 | 1.00 | 23.98 |
| | ATOM | 3619 | O | GLU | B | 523 | -5.993 | -7.616 | 11.147 | 1.00 | 22.08 |
| | ATOM | 3620 | N | HIS | B | 524 | -4.187 | -8.287 | 12.326 | 1.00 | 23.46 |
| | ATOM | 3621 | CA | HIS | B | 524 | -4.846 | -9.428 | 12.952 | 1.00 | 26.20 |
| | ATOM | 3622 | CB | HIS | B | 524 | -3.824 | -10.245 | 13.743 | 1.00 | 27.26 |
| 50 | ATOM | 3623 | CG | HIS | B | 524 | -4.378 | -11.509 | 14.321 | 1.00 | 30.91 |
| | ATOM | 3624 | CD2 | HIS | B | 524 | -4.308 | -12.792 | 13.892 | 1.00 | 30.90 |
| | ATOM | 3625 | ND1 | HIS | B | 524 | -5.107 | -11.537 | 15.490 | 1.00 | 28.87 |
| | ATOM | 3626 | CE1 | HIS | B | 524 | -5.461 | -12.780 | 15.757 | 1.00 | 30.45 |
| | ATOM | 3627 | NE2 | HIS | B | 524 | -4.989 | -13.561 | 14.803 | 1.00 | 29.19 |
| 55 | ATOM | 3628 | C | HIS | B | 524 | -5.996 | -9.025 | 13.870 | 1.00 | 27.69 |
| | ATOM | 3629 | O | HIS | B | 524 | -7.061 | -9.656 | 13.860 | 1.00 | 25.00 |
| | ATOM | 3630 | N | LEU | B | 525 | -5.777 | -7.977 | 14.655 | 1.00 | 23.84 |
| | ATOM | 3631 | CA | LEU | B | 525 | -6.786 | -7.492 | 15.588 | 1.00 | 25.77 |
| | ATOM | 3632 | CB | LEU | B | 525 | -6.217 | -6.358 | 16.444 | 1.00 | 22.22 |
| 60 | ATOM | 3633 | CG | LEU | B | 525 | -7.164 | -5.778 | 17.498 | 1.00 | 26.81 |
| | ATOM | 3634 | CD1 | LEU | B | 525 | -7.763 | -6.922 | 18.321 | 1.00 | 23.32 |

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|----|------|------|-----|-----|---|-----|---------|---------|--------|------|-------|
| 5 | ATOM | 3635 | CD2 | LEU | B | 525 | -6.414 | -4.793 | 18.399 | 1.00 | 18.95 |
| | ATOM | 3636 | C | LEU | B | 525 | -8.013 | -6.995 | 14.842 | 1.00 | 26.84 |
| | ATOM | 3637 | O | LEU | B | 525 | -9.154 | -7.247 | 15.249 | 1.00 | 26.73 |
| | ATOM | 3638 | N | TYR | B | 526 | -7.764 | -6.271 | 13.757 | 1.00 | 26.86 |
| | ATOM | 3639 | CA | TYR | B | 526 | -8.819 | -5.726 | 12.918 | 1.00 | 30.89 |
| 10 | ATOM | 3640 | CB | TYR | B | 526 | -8.201 | -4.818 | 11.854 | 1.00 | 34.31 |
| | ATOM | 3641 | CG | TYR | B | 526 | -9.183 | -4.223 | 10.878 | 1.00 | 43.50 |
| | ATOM | 3642 | CD1 | TYR | B | 526 | -10.058 | -3.211 | 11.267 | 1.00 | 47.66 |
| | ATOM | 3643 | CE1 | TYR | B | 526 | -10.943 | -2.636 | 10.357 | 1.00 | 48.85 |
| | ATOM | 3644 | CD2 | TYR | B | 526 | -9.218 | -4.651 | 9.552 | 1.00 | 48.52 |
| 15 | ATOM | 3645 | CE2 | TYR | B | 526 | -10.098 | -4.083 | 8.634 | 1.00 | 52.43 |
| | ATOM | 3646 | CZ | TYR | B | 526 | -10.955 | -3.077 | 9.043 | 1.00 | 51.67 |
| | ATOM | 3647 | OH | TYR | B | 526 | -11.810 | -2.504 | 8.129 | 1.00 | 57.01 |
| | ATOM | 3648 | C | TYR | B | 526 | -9.577 | -6.880 | 12.265 | 1.00 | 30.90 |
| | ATOM | 3649 | O | TYR | B | 526 | -10.793 | -6.829 | 12.113 | 1.00 | 31.48 |
| 20 | ATOM | 3650 | N | SER | B | 527 | -8.849 | -7.926 | 11.889 | 1.00 | 31.39 |
| | ATOM | 3651 | CA | SER | B | 527 | -9.460 | -9.095 | 11.266 | 1.00 | 33.73 |
| | ATOM | 3652 | CB | SER | B | 527 | -8.377 | -10.048 | 10.749 | 1.00 | 34.13 |
| | ATOM | 3653 | OG | SER | B | 527 | -8.945 | -11.222 | 10.196 | 1.00 | 43.67 |
| | ATOM | 3654 | C | SER | B | 527 | -10.339 | -9.813 | 12.288 | 1.00 | 34.34 |
| 25 | ATOM | 3655 | O | SER | B | 527 | -11.446 | -10.261 | 11.973 | 1.00 | 33.42 |
| | ATOM | 3656 | N | MET | B | 528 | -9.840 | -9.916 | 13.517 | 1.00 | 31.66 |
| | ATOM | 3657 | CA | MET | B | 528 | -10.574 | -10.572 | 14.589 | 1.00 | 29.77 |
| | ATOM | 3658 | CB | MET | B | 528 | -9.682 | -10.743 | 15.820 | 1.00 | 32.96 |
| | ATOM | 3659 | CG | MET | B | 528 | -8.651 | -11.859 | 15.699 | 1.00 | 33.47 |
| 30 | ATOM | 3660 | SD | MET | B | 528 | -9.359 | -13.427 | 15.134 | 1.00 | 38.28 |
| | ATOM | 3661 | CE | MET | B | 528 | -10.265 | -13.915 | 16.579 | 1.00 | 36.01 |
| | ATOM | 3662 | C | MET | B | 528 | -11.800 | -9.747 | 14.953 | 1.00 | 29.42 |
| | ATOM | 3663 | O | MET | B | 528 | -12.835 | -10.293 | 15.331 | 1.00 | 28.65 |
| | ATOM | 3664 | N | LYS | B | 529 | -11.673 | -8.429 | 14.850 | 1.00 | 30.64 |
| 35 | ATOM | 3665 | CA | LYS | B | 529 | -12.781 | -7.533 | 15.149 | 1.00 | 31.80 |
| | ATOM | 3666 | CB | LYS | B | 529 | -12.323 | -6.079 | 15.027 | 1.00 | 32.86 |
| | ATOM | 3667 | CG | LYS | B | 529 | -13.436 | -5.043 | 15.114 | 1.00 | 36.42 |
| | ATOM | 3668 | CD | LYS | B | 529 | -13.114 | -3.852 | 14.224 | 1.00 | 41.74 |
| | ATOM | 3669 | CE | LYS | B | 529 | -13.734 | -2.564 | 14.741 | 1.00 | 43.45 |
| 40 | ATOM | 3670 | NZ | LYS | B | 529 | -15.221 | -2.569 | 14.634 | 1.00 | 46.51 |
| | ATOM | 3671 | C | LYS | B | 529 | -13.857 | -7.840 | 14.116 | 1.00 | 36.60 |
| | ATOM | 3672 | O | LYS | B | 529 | -15.049 | -7.877 | 14.424 | 1.00 | 34.04 |
| | ATOM | 3673 | N | CYS | B | 530 | -13.407 | -8.083 | 12.889 | 1.00 | 40.04 |
| | ATOM | 3674 | CA | CYS | B | 530 | -14.286 | -8.409 | 11.773 | 1.00 | 44.58 |
| 45 | ATOM | 3675 | CB | CYS | B | 530 | -13.460 | -8.535 | 10.491 | 1.00 | 50.64 |
| | ATOM | 3676 | SG | CYS | B | 530 | -13.369 | -7.034 | 9.504 | 1.00 | 67.65 |
| | ATOM | 3677 | C | CYS | B | 530 | -15.065 | -9.692 | 12.016 | 1.00 | 42.88 |
| | ATOM | 3678 | O | CYS | B | 530 | -16.274 | -9.741 | 11.807 | 1.00 | 40.15 |
| | ATOM | 3679 | N | LYS | B | 531 | -14.360 | -10.733 | 12.447 | 1.00 | 41.92 |
| 50 | ATOM | 3680 | CA | LYS | B | 531 | -14.980 | -12.023 | 12.728 | 1.00 | 42.60 |
| | ATOM | 3681 | CB | LYS | B | 531 | -13.907 | -13.091 | 12.927 | 1.00 | 44.77 |
| | ATOM | 3682 | C | LYS | B | 531 | -15.844 | -11.907 | 13.977 | 1.00 | 44.43 |
| | ATOM | 3683 | O | LYS | B | 531 | -16.623 | -12.804 | 14.296 | 1.00 | 44.09 |
| | ATOM | 3684 | N | ASN | B | 532 | -15.678 | -10.793 | 14.685 | 1.00 | 44.98 |
| 55 | ATOM | 3685 | CA | ASN | B | 532 | -16.437 | -10.496 | 15.893 | 1.00 | 44.10 |
| | ATOM | 3686 | CB | ASN | B | 532 | -17.833 | -10.003 | 15.506 | 1.00 | 45.14 |
| | ATOM | 3687 | CG | ASN | B | 532 | -18.526 | -9.271 | 16.633 | 1.00 | 46.54 |
| | ATOM | 3688 | OD1 | ASN | B | 532 | -19.729 | -9.424 | 16.837 | 1.00 | 50.62 |
| | ATOM | 3689 | ND2 | ASN | B | 532 | -17.771 | -8.471 | 17.375 | 1.00 | 46.07 |
| 60 | ATOM | 3690 | C | ASN | B | 532 | -16.557 | -11.657 | 16.882 | 1.00 | 43.34 |
| | ATOM | 3691 | O | ASN | B | 532 | -17.655 | -11.994 | 17.321 | 1.00 | 41.42 |

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|----|------|------|-----|-----|---|-----|---------|---------|--------|------|-------|
| 5 | ATOM | 3692 | N | VAL | B | 533 | -15.434 | -12.264 | 17.243 | 1.00 | 43.45 |
| | ATOM | 3693 | CA | VAL | B | 533 | -15.471 | -13.371 | 18.190 | 1.00 | 44.06 |
| | ATOM | 3694 | CB | VAL | B | 533 | -14.170 | -14.219 | 18.120 | 1.00 | 45.56 |
| | ATOM | 3695 | CG1 | VAL | B | 533 | -13.661 | -14.263 | 16.683 | 1.00 | 45.67 |
| | ATOM | 3696 | CG2 | VAL | B | 533 | -13.107 | -13.644 | 19.045 | 1.00 | 44.16 |
| 10 | ATOM | 3697 | C | VAL | B | 533 | -15.670 | -12.835 | 19.611 | 1.00 | 43.24 |
| | ATOM | 3698 | O | VAL | B | 533 | -15.894 | -13.602 | 20.548 | 1.00 | 44.21 |
| | ATOM | 3699 | N | VAL | B | 534 | -15.596 | -11.511 | 19.755 | 1.00 | 40.44 |
| | ATOM | 3700 | CA | VAL | B | 534 | -15.765 | -10.849 | 21.049 | 1.00 | 37.80 |
| | ATOM | 3701 | CB | VAL | B | 534 | -14.630 | -11.259 | 22.038 | 1.00 | 36.38 |
| 15 | ATOM | 3702 | CG1 | VAL | B | 534 | -13.324 | -10.575 | 21.658 | 1.00 | 34.35 |
| | ATOM | 3703 | CG2 | VAL | B | 534 | -15.021 | -10.910 | 23.463 | 1.00 | 39.34 |
| | ATOM | 3704 | C | VAL | B | 534 | -15.752 | -9.329 | 20.857 | 1.00 | 37.97 |
| | ATOM | 3705 | O | VAL | B | 534 | -15.026 | -8.808 | 20.008 | 1.00 | 39.45 |
| | ATOM | 3706 | N | PRO | B | 535 | -16.575 | -8.597 | 21.625 | 1.00 | 37.81 |
| 20 | ATOM | 3707 | CD | PRO | B | 535 | -17.529 | -9.078 | 22.640 | 1.00 | 38.74 |
| | ATOM | 3708 | CA | PRO | B | 535 | -16.608 | -7.135 | 21.492 | 1.00 | 36.79 |
| | ATOM | 3709 | CB | PRO | B | 535 | -17.846 | -6.729 | 22.288 | 1.00 | 36.98 |
| | ATOM | 3710 | CG | PRO | B | 535 | -18.004 | -7.809 | 23.298 | 1.00 | 39.77 |
| | ATOM | 3711 | C | PRO | B | 535 | -15.338 | -6.494 | 22.049 | 1.00 | 33.95 |
| 25 | ATOM | 3712 | O | PRO | B | 535 | -14.786 | -6.963 | 23.040 | 1.00 | 34.93 |
| | ATOM | 3713 | N | LEU | B | 536 | -14.881 | -5.426 | 21.409 | 1.00 | 33.42 |
| | ATOM | 3714 | CA | LEU | B | 536 | -13.675 | -4.732 | 21.851 | 1.00 | 33.40 |
| | ATOM | 3715 | CB | LEU | B | 536 | -12.829 | -4.314 | 20.647 | 1.00 | 29.31 |
| | ATOM | 3716 | CG | LEU | B | 536 | -12.219 | -5.433 | 19.798 | 1.00 | 30.06 |
| 30 | ATOM | 3717 | CD1 | LEU | B | 536 | -11.344 | -4.822 | 18.714 | 1.00 | 30.85 |
| | ATOM | 3718 | CD2 | LEU | B | 536 | -11.398 | -6.370 | 20.676 | 1.00 | 28.96 |
| | ATOM | 3719 | C | LEU | B | 536 | -14.036 | -3.498 | 22.666 | 1.00 | 30.50 |
| | ATOM | 3720 | O | LEU | B | 536 | -15.024 | -2.829 | 22.383 | 1.00 | 29.91 |
| | ATOM | 3721 | N | TYR | B | 537 | -13.231 | -3.194 | 23.676 | 1.00 | 28.69 |
| 35 | ATOM | 3722 | CA | TYR | B | 537 | -13.494 | -2.032 | 24.505 | 1.00 | 29.89 |
| | ATOM | 3723 | CB | TYR | B | 537 | -12.618 | -2.071 | 25.750 | 1.00 | 32.50 |
| | ATOM | 3724 | CG | TYR | B | 537 | -12.849 | -3.327 | 26.543 | 1.00 | 39.46 |
| | ATOM | 3725 | CD1 | TYR | B | 537 | -13.923 | -3.431 | 27.421 | 1.00 | 41.90 |
| | ATOM | 3726 | CE1 | TYR | B | 537 | -14.174 | -4.609 | 28.118 | 1.00 | 45.72 |
| 40 | ATOM | 3727 | CD2 | TYR | B | 537 | -12.022 | -4.435 | 26.379 | 1.00 | 47.39 |
| | ATOM | 3728 | CE2 | TYR | B | 537 | -12.262 | -5.620 | 27.072 | 1.00 | 49.93 |
| | ATOM | 3729 | CZ | TYR | B | 537 | -13.340 | -5.699 | 27.940 | 1.00 | 48.80 |
| | ATOM | 3730 | OH | TYR | B | 537 | -13.582 | -6.872 | 28.624 | 1.00 | 53.90 |
| | ATOM | 3731 | C | TYR | B | 537 | -13.262 | -0.761 | 23.709 | 1.00 | 27.09 |
| 45 | ATOM | 3732 | O | TYR | B | 537 | -12.518 | -0.757 | 22.729 | 1.00 | 26.15 |
| | ATOM | 3733 | N | ASP | B | 538 | -13.909 | 0.315 | 24.141 | 1.00 | 26.12 |
| | ATOM | 3734 | CA | ASP | B | 538 | -13.830 | 1.598 | 23.461 | 1.00 | 25.27 |
| | ATOM | 3735 | CB | ASP | B | 538 | -14.748 | 2.598 | 24.164 | 1.00 | 28.85 |
| | ATOM | 3736 | CG | ASP | B | 538 | -16.227 | 2.285 | 23.940 | 1.00 | 33.90 |
| 50 | ATOM | 3737 | OD1 | ASP | B | 538 | -17.052 | 2.613 | 24.819 | 1.00 | 32.68 |
| | ATOM | 3738 | OD2 | ASP | B | 538 | -16.562 | 1.707 | 22.882 | 1.00 | 38.26 |
| | ATOM | 3739 | C | ASP | B | 538 | -12.447 | 2.217 | 23.261 | 1.00 | 25.18 |
| | ATOM | 3740 | O | ASP | B | 538 | -12.120 | 2.626 | 22.147 | 1.00 | 26.41 |
| | ATOM | 3741 | N | LEU | B | 539 | -11.637 | 2.309 | 24.313 | 1.00 | 20.76 |
| 55 | ATOM | 3742 | CA | LEU | B | 539 | -10.312 | 2.911 | 24.150 | 1.00 | 19.65 |
| | ATOM | 3743 | CB | LEU | B | 539 | -9.567 | 2.991 | 25.496 | 1.00 | 17.48 |
| | ATOM | 3744 | CG | LEU | B | 539 | -8.116 | 3.511 | 25.469 | 1.00 | 16.46 |
| | ATOM | 3745 | CD1 | LEU | B | 539 | -8.051 | 4.892 | 24.838 | 1.00 | 16.43 |
| | ATOM | 3746 | CD2 | LEU | B | 539 | -7.564 | 3.569 | 26.895 | 1.00 | 15.57 |
| 60 | ATOM | 3747 | C | LEU | B | 539 | -9.484 | 2.127 | 23.127 | 1.00 | 16.75 |
| | ATOM | 3748 | O | LEU | B | 539 | -8.862 | 2.716 | 22.249 | 1.00 | 20.36 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|
| 5 | ATOM | 3749 | N | LEU | B | 540 | -9.487 | 0.803 | 23.239 | 1.00 | 18.23 |
| | ATOM | 3750 | CA | LEU | B | 540 | -8.743 | -0.048 | 22.319 | 1.00 | 18.05 |
| | ATOM | 3751 | CB | LEU | B | 540 | -8.909 | -1.528 | 22.701 | 1.00 | 16.38 |
| | ATOM | 3752 | CG | LEU | B | 540 | -8.188 | -2.554 | 21.821 | 1.00 | 19.81 |
| | ATOM | 3753 | CD1 | LEU | B | 540 | -6.679 | -2.303 | 21.828 | 1.00 | 19.27 |
| 10 | ATOM | 3754 | CD2 | LEU | B | 540 | -8.473 | -3.952 | 22.327 | 1.00 | 18.00 |
| | ATOM | 3755 | C | LEU | B | 540 | -9.241 | 0.169 | 20.891 | 1.00 | 21.50 |
| | ATOM | 3756 | O | LEU | B | 540 | -8.449 | 0.293 | 19.964 | 1.00 | 20.41 |
| | ATOM | 3757 | N | LEU | B | 541 | -10.559 | 0.206 | 20.726 | 1.00 | 22.40 |
| | ATOM | 3758 | CA | LEU | B | 541 | -11.164 | 0.419 | 19.413 | 1.00 | 23.27 |
| 15 | ATOM | 3759 | CB | LEU | B | 541 | -12.686 | 0.429 | 19.527 | 1.00 | 25.12 |
| | ATOM | 3760 | CG | LEU | B | 541 | -13.410 | -0.808 | 18.999 | 1.00 | 36.53 |
| | ATOM | 3761 | CD1 | LEU | B | 541 | -14.910 | -0.671 | 19.273 | 1.00 | 30.98 |
| | ATOM | 3762 | CD2 | LEU | B | 541 | -13.136 | -0.971 | 17.508 | 1.00 | 31.93 |
| | ATOM | 3763 | C | LEU | B | 541 | -10.697 | 1.751 | 18.842 | 1.00 | 22.46 |
| 20 | ATOM | 3764 | O | LEU | B | 541 | -10.359 | 1.845 | 17.666 | 1.00 | 26.29 |
| | ATOM | 3765 | N | GLU | B | 542 | -10.694 | 2.781 | 19.680 | 1.00 | 23.96 |
| | ATOM | 3766 | CA | GLU | B | 542 | -10.248 | 4.106 | 19.270 | 1.00 | 26.91 |
| | ATOM | 3767 | CB | GLU | B | 542 | -10.250 | 5.050 | 20.468 | 1.00 | 30.84 |
| | ATOM | 3768 | CG | GLU | B | 542 | -11.166 | 6.245 | 20.347 | 1.00 | 37.20 |
| 25 | ATOM | 3769 | CD | GLU | B | 542 | -11.138 | 7.105 | 21.597 | 1.00 | 39.98 |
| | ATOM | 3770 | OE1 | GLU | B | 542 | -12.223 | 7.385 | 22.144 | 1.00 | 39.92 |
| | ATOM | 3771 | OE2 | GLU | B | 542 | -10.028 | 7.494 | 22.034 | 1.00 | 38.96 |
| | ATOM | 3772 | C | GLU | B | 542 | -8.826 | 4.010 | 18.724 | 1.00 | 27.90 |
| | ATOM | 3773 | O | GLU | B | 542 | -8.530 | 4.492 | 17.634 | 1.00 | 29.32 |
| 30 | ATOM | 3774 | N | MET | B | 543 | -7.945 | 3.388 | 19.499 | 1.00 | 26.41 |
| | ATOM | 3775 | CA | MET | B | 543 | -6.552 | 3.237 | 19.107 | 1.00 | 23.53 |
| | ATOM | 3776 | CB | MET | B | 543 | -5.749 | 2.591 | 20.247 | 1.00 | 24.60 |
| | ATOM | 3777 | CG | MET | B | 543 | -5.812 | 3.338 | 21.579 | 1.00 | 26.46 |
| | ATOM | 3778 | SD | MET | B | 543 | -5.373 | 5.084 | 21.467 | 1.00 | 29.45 |
| 35 | ATOM | 3779 | CE | MET | B | 543 | -3.585 | 4.971 | 21.349 | 1.00 | 25.43 |
| | ATOM | 3780 | C | MET | B | 543 | -6.403 | 2.407 | 17.832 | 1.00 | 25.80 |
| | ATOM | 3781 | O | MET | B | 543 | -5.535 | 2.686 | 17.004 | 1.00 | 23.59 |
| | ATOM | 3782 | N | LEU | B | 544 | -7.254 | 1.394 | 17.673 | 1.00 | 27.74 |
| | ATOM | 3783 | CA | LEU | B | 544 | -7.202 | 0.522 | 16.499 | 1.00 | 26.32 |
| 40 | ATOM | 3784 | CB | LEU | B | 544 | -8.069 | -0.721 | 16.719 | 1.00 | 26.75 |
| | ATOM | 3785 | CG | LEU | B | 544 | -8.274 | -1.632 | 15.502 | 1.00 | 28.12 |
| | ATOM | 3786 | CD1 | LEU | B | 544 | -6.956 | -2.294 | 15.136 | 1.00 | 26.36 |
| | ATOM | 3787 | CD2 | LEU | B | 544 | -9.330 | -2.680 | 15.803 | 1.00 | 27.00 |
| | ATOM | 3788 | C | LEU | B | 544 | -7.672 | 1.252 | 15.250 | 1.00 | 26.97 |
| 45 | ATOM | 3789 | O | LEU | B | 544 | -7.036 | 1.181 | 14.195 | 1.00 | 24.25 |
| | ATOM | 3790 | N | ASP | B | 545 | -8.787 | 1.961 | 15.372 | 1.00 | 30.37 |
| | ATOM | 3791 | CA | ASP | B | 545 | -9.338 | 2.702 | 14.244 | 1.00 | 32.34 |
| | ATOM | 3792 | CB | ASP | B | 545 | -10.668 | 3.346 | 14.637 | 1.00 | 36.61 |
| | ATOM | 3793 | CG | ASP | B | 545 | -11.818 | 2.370 | 14.565 | 1.00 | 42.73 |
| 50 | ATOM | 3794 | OD1 | ASP | B | 545 | -12.858 | 2.624 | 15.211 | 1.00 | 47.39 |
| | ATOM | 3795 | OD2 | ASP | B | 545 | -11.676 | 1.342 | 13.863 | 1.00 | 46.96 |
| | ATOM | 3796 | C | ASP | B | 545 | -8.382 | 3.762 | 13.711 | 1.00 | 31.27 |
| | ATOM | 3797 | O | ASP | B | 545 | -8.443 | 4.120 | 12.532 | 1.00 | 30.53 |
| | ATOM | 3798 | N | ALA | B | 546 | -7.506 | 4.272 | 14.572 | 1.00 | 29.02 |
| 55 | ATOM | 3799 | CA | ALA | B | 546 | -6.543 | 5.280 | 14.141 | 1.00 | 31.21 |
| | ATOM | 3800 | CB | ALA | B | 546 | -5.646 | 5.693 | 15.306 | 1.00 | 30.98 |
| | ATOM | 3801 | C | ALA | B | 546 | -5.697 | 4.731 | 12.996 | 1.00 | 32.14 |
| | ATOM | 3802 | O | ALA | B | 546 | -5.189 | 5.490 | 12.170 | 1.00 | 33.78 |
| | ATOM | 3803 | N | HIS | B | 547 | -5.555 | 3.410 | 12.943 | 1.00 | 32.27 |
| 60 | ATOM | 3804 | CA | HIS | B | 547 | -4.773 | 2.767 | 11.892 | 1.00 | 37.73 |
| | ATOM | 3805 | CB | HIS | B | 547 | -3.991 | 1.576 | 12.457 | 1.00 | 35.83 |

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|----|--------|------|-----|-----|---|-----|---------|---------|--------|------|-------|
| 5 | ATOM | 3806 | CG | HIS | B | 547 | -2.796 | 1.968 | 13.269 | 1.00 | 34.54 |
| | ATOM | 3807 | CD2 | HIS | B | 547 | -2.698 | 2.553 | 14.486 | 1.00 | 30.23 |
| | ATOM | 3808 | ND1 | HIS | B | 547 | -1.502 | 1.755 | 12.840 | 1.00 | 34.23 |
| | ATOM | 3809 | CE1 | HIS | B | 547 | -0.659 | 2.193 | 13.760 | 1.00 | 36.72 |
| | ATOM | 3810 | NE2 | HIS | B | 547 | -1.360 | 2.681 | 14.768 | 1.00 | 31.48 |
| 10 | ATOM | 3811 | C | HIS | B | 547 | -5.649 | 2.286 | 10.735 | 1.00 | 43.69 |
| | ATOM | 3812 | O | HIS | B | 547 | -5.178 | 2.152 | 9.606 | 1.00 | 46.04 |
| | ATOM | 3813 | N | ARG | B | 548 | -6.919 | 2.020 | 11.019 | 1.00 | 48.35 |
| | ATOM | 3814 | CA | ARG | B | 548 | -7.843 | 1.551 | 9.993 | 1.00 | 54.74 |
| | ATOM | 3815 | CB | ARG | B | 548 | -8.522 | 0.267 | 10.452 | 1.00 | 54.66 |
| 15 | ATOM | 3816 | C | ARG | B | 548 | -8.886 | 2.619 | 9.681 | 1.00 | 59.94 |
| | ATOM | 3817 | O | ARG | B | 548 | -8.580 | 3.812 | 9.672 | 1.00 | 62.81 |
| | ATOM | 3818 | N | LEU | B | 549 | -10.116 | 2.186 | 9.422 | 1.00 | 64.81 |
| | ATOM | 3819 | CA | LEU | B | 549 | -11.204 | 3.109 | 9.112 | 1.00 | 67.59 |
| | ATOM | 3820 | CB | LEU | B | 549 | -12.478 | 2.327 | 8.799 | 1.00 | 68.06 |
| 20 | ATOM | 3821 | C | LEU | B | 549 | -11.449 | 4.069 | 10.275 | 1.00 | 69.12 |
| | ATOM | 3822 | O | LEU | B | 549 | -11.451 | 5.297 | 10.036 | 1.00 | 68.96 |
| | ATOM | 3823 | OXT | LEU | B | 549 | -11.634 | 3.579 | 11.412 | 1.00 | 70.70 |
| | HETATM | 3824 | CP9 | DES | B | 600 | -4.547 | -6.077 | 22.000 | 1.00 | 18.55 |
| | HETATM | 3825 | CP8 | DES | B | 600 | -3.163 | -6.365 | 21.467 | 1.00 | 17.72 |
| 25 | HETATM | 3826 | CP7 | DES | B | 600 | -2.897 | -7.853 | 21.381 | 1.00 | 21.17 |
| | HETATM | 3827 | CP6 | DES | B | 600 | -3.719 | -8.551 | 20.374 | 1.00 | 22.05 |
| | HETATM | 3828 | CP1 | DES | B | 600 | -3.405 | -8.481 | 18.998 | 1.00 | 21.32 |
| | HETATM | 3829 | CP2 | DES | B | 600 | -4.239 | -9.095 | 18.063 | 1.00 | 21.61 |
| | HETATM | 3830 | CP3 | DES | B | 600 | -5.388 | -9.771 | 18.509 | 1.00 | 24.89 |
| 30 | HETATM | 3831 | OP3 | DES | B | 600 | -6.244 | -10.339 | 17.600 | 1.00 | 24.94 |
| | HETATM | 3832 | CP4 | DES | B | 600 | -5.718 | -9.858 | 19.860 | 1.00 | 24.08 |
| | HETATM | 3833 | CP5 | DES | B | 600 | -4.877 | -9.240 | 20.791 | 1.00 | 24.67 |
| | HETATM | 3834 | C7 | DES | B | 600 | -1.998 | -8.460 | 22.190 | 1.00 | 16.67 |
| | HETATM | 3835 | C6 | DES | B | 600 | -1.330 | -7.834 | 23.325 | 1.00 | 15.39 |
| 35 | HETATM | 3836 | C5 | DES | B | 600 | -2.054 | -7.642 | 24.522 | 1.00 | 17.62 |
| | HETATM | 3837 | C4 | DES | B | 600 | -1.433 | -7.072 | 25.634 | 1.00 | 16.16 |
| | HETATM | 3838 | C3 | DES | B | 600 | -0.077 | -6.685 | 25.542 | 1.00 | 20.04 |
| | HETATM | 3839 | O3 | DES | B | 600 | 0.509 | -6.113 | 26.655 | 1.00 | 15.55 |
| | HETATM | 3840 | C2 | DES | B | 600 | 0.669 | -6.866 | 24.353 | 1.00 | 18.94 |
| 40 | HETATM | 3841 | C1 | DES | B | 600 | 0.035 | -7.440 | 23.241 | 1.00 | 15.20 |
| | HETATM | 3842 | C8 | DES | B | 600 | -1.642 | -9.903 | 21.942 | 1.00 | 17.61 |
| | HETATM | 3843 | C9 | DES | B | 600 | -0.440 | -10.009 | 20.998 | 1.00 | 11.63 |
| | HETATM | 3844 | C1 | CBM | B | 417 | -4.997 | -22.994 | 25.273 | 1.00 | 55.80 |
| | HETATM | 3845 | O4 | CBM | B | 417 | -4.789 | -24.187 | 25.003 | 1.00 | 55.56 |
| 45 | HETATM | 3846 | O3 | CBM | B | 417 | -4.798 | -22.559 | 26.552 | 1.00 | 56.04 |
| | HETATM | 3847 | C2 | CBM | B | 417 | -5.468 | -21.960 | 24.264 | 1.00 | 57.04 |
| | HETATM | 3848 | C1 | CBM | B | 530 | -15.278 | -5.124 | 10.243 | 1.00 | 87.39 |
| | HETATM | 3849 | O4 | CBM | B | 530 | -15.852 | -5.086 | 9.064 | 1.00 | 87.68 |
| | HETATM | 3850 | O3 | CBM | B | 530 | -15.832 | -4.291 | 11.201 | 1.00 | 86.22 |
| 50 | HETATM | 3851 | C2 | CBM | B | 530 | -14.207 | -5.886 | 10.628 | 1.00 | 87.65 |
| | ATOM | 3852 | CB | HIS | C | 687 | 9.818 | -20.030 | -2.211 | 1.00 | 63.34 |
| | ATOM | 3853 | C | HIS | C | 687 | 10.133 | -20.267 | -4.689 | 1.00 | 63.49 |
| | ATOM | 3854 | O | HIS | C | 687 | 11.204 | -20.840 | -4.472 | 1.00 | 63.87 |
| | ATOM | 3855 | N | HIS | C | 687 | 7.944 | -19.563 | -3.758 | 1.00 | 65.42 |
| 55 | ATOM | 3856 | CA | HIS | C | 687 | 9.424 | -19.484 | -3.586 | 1.00 | 64.86 |
| | ATOM | 3857 | N | LYS | C | 688 | 9.533 | -20.281 | -5.875 | 1.00 | 62.00 |
| | ATOM | 3858 | CA | LYS | C | 688 | 10.101 | -20.999 | -7.009 | 1.00 | 60.81 |
| | ATOM | 3859 | CB | LYS | C | 688 | 8.980 | -21.540 | -7.901 | 1.00 | 61.76 |
| | ATOM | 3860 | C | LYS | C | 688 | 11.050 | -20.127 | -7.827 | 1.00 | 57.47 |
| 60 | ATOM | 3861 | O | LYS | C | 688 | 12.253 | -20.379 | -7.858 | 1.00 | 57.64 |
| | ATOM | 3862 | N | ILE | C | 689 | 10.511 | -19.103 | -8.482 | 1.00 | 55.74 |

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|----|------|------|-----|-----|---|-----|--------|---------|---------|------|-------|
| 5 | ATOM | 3863 | CA | ILE | C | 689 | 11.326 | -18.212 | -9.306 | 1.00 | 53.09 |
| | ATOM | 3864 | CB | ILE | C | 689 | 10.496 | -17.057 | -9.889 | 1.00 | 53.83 |
| | ATOM | 3865 | CG2 | ILE | C | 689 | 11.334 | -16.286 | -10.902 | 1.00 | 54.55 |
| | ATOM | 3866 | CG1 | ILE | C | 689 | 9.229 | -17.603 | -10.551 | 1.00 | 52.90 |
| | ATOM | 3867 | CD1 | ILE | C | 689 | 8.406 | -16.550 | -11.258 | 1.00 | 50.45 |
| 10 | ATOM | 3868 | C | ILE | C | 689 | 12.513 | -17.611 | -8.560 | 1.00 | 50.82 |
| | ATOM | 3869 | O | ILE | C | 689 | 13.616 | -17.550 | -9.097 | 1.00 | 51.28 |
| | ATOM | 3870 | N | LEU | C | 690 | 12.288 | -17.162 | -7.329 | 1.00 | 48.01 |
| | ATOM | 3871 | CA | LEU | C | 690 | 13.362 | -16.570 | -6.534 | 1.00 | 47.33 |
| | ATOM | 3872 | CB | LEU | C | 690 | 12.812 | -16.058 | -5.199 | 1.00 | 42.51 |
| 15 | ATOM | 3873 | CG | LEU | C | 690 | 13.835 | -15.501 | -4.206 | 1.00 | 40.67 |
| | ATOM | 3874 | CD1 | LEU | C | 690 | 14.575 | -14.324 | -4.831 | 1.00 | 39.95 |
| | ATOM | 3875 | CD2 | LEU | C | 690 | 13.128 | -15.078 | -2.926 | 1.00 | 38.77 |
| | ATOM | 3876 | C | LEU | C | 690 | 14.445 | -17.615 | -6.282 | 1.00 | 48.87 |
| | ATOM | 3877 | O | LEU | C | 690 | 15.643 | -17.340 | -6.393 | 1.00 | 46.71 |
| 20 | ATOM | 3878 | N | HIS | C | 691 | 14.001 | -18.818 | -5.939 | 1.00 | 51.36 |
| | ATOM | 3879 | CA | HIS | C | 691 | 14.886 | -19.946 | -5.675 | 1.00 | 53.35 |
| | ATOM | 3880 | CB | HIS | C | 691 | 14.042 | -21.203 | -5.460 | 1.00 | 58.64 |
| | ATOM | 3881 | CG | HIS | C | 691 | 14.655 | -22.195 | -4.526 | 1.00 | 62.94 |
| | ATOM | 3882 | CD2 | HIS | C | 691 | 15.503 | -23.227 | -4.751 | 1.00 | 64.95 |
| 25 | ATOM | 3883 | ND1 | HIS | C | 691 | 14.392 | -22.202 | -3.173 | 1.00 | 65.49 |
| | ATOM | 3884 | CE1 | HIS | C | 691 | 15.053 | -23.195 | -2.605 | 1.00 | 68.18 |
| | ATOM | 3885 | NE2 | HIS | C | 691 | 15.733 | -23.833 | -3.540 | 1.00 | 68.77 |
| | ATOM | 3886 | C | HIS | C | 691 | 15.824 | -20.162 | -6.861 | 1.00 | 52.19 |
| | ATOM | 3887 | O | HIS | C | 691 | 17.048 | -20.153 | -6.717 | 1.00 | 47.53 |
| 30 | ATOM | 3888 | N | ARG | C | 692 | 15.222 | -20.350 | -8.032 | 1.00 | 52.37 |
| | ATOM | 3889 | CA | ARG | C | 692 | 15.949 | -20.586 | -9.271 | 1.00 | 52.90 |
| | ATOM | 3890 | CB | ARG | C | 692 | 14.955 | -20.832 | -10.410 | 1.00 | 54.04 |
| | ATOM | 3891 | CG | ARG | C | 692 | 15.575 | -20.826 | -11.797 | 1.00 | 57.52 |
| | ATOM | 3892 | CD | ARG | C | 692 | 14.528 | -21.048 | -12.874 | 1.00 | 58.25 |
| 35 | ATOM | 3893 | NE | ARG | C | 692 | 14.375 | -19.878 | -13.732 | 1.00 | 61.43 |
| | ATOM | 3894 | CZ | ARG | C | 692 | 13.218 | -19.260 | -13.951 | 1.00 | 64.32 |
| | ATOM | 3895 | NH1 | ARG | C | 692 | 12.108 | -19.706 | -13.378 | 1.00 | 63.22 |
| | ATOM | 3896 | NH2 | ARG | C | 692 | 13.171 | -18.197 | -14.746 | 1.00 | 65.93 |
| | ATOM | 3897 | C | ARG | C | 692 | 16.873 | -19.434 | -9.639 | 1.00 | 53.09 |
| 40 | ATOM | 3898 | O | ARG | C | 692 | 18.047 | -19.644 | -9.956 | 1.00 | 53.06 |
| | ATOM | 3899 | N | LEU | C | 693 | 16.338 | -18.217 | -9.607 | 1.00 | 50.73 |
| | ATOM | 3900 | CA | LEU | C | 693 | 17.125 | -17.039 | -9.945 | 1.00 | 49.53 |
| | ATOM | 3901 | CB | LEU | C | 693 | 16.249 | -15.784 | -9.881 | 1.00 | 49.56 |
| | ATOM | 3902 | CG | LEU | C | 693 | 15.781 | -15.245 | -11.239 | 1.00 | 49.78 |
| 45 | ATOM | 3903 | CD1 | LEU | C | 693 | 15.219 | -16.389 | -12.079 | 1.00 | 50.30 |
| | ATOM | 3904 | CD2 | LEU | C | 693 | 14.728 | -14.170 | -11.037 | 1.00 | 48.79 |
| | ATOM | 3905 | C | LEU | C | 693 | 18.318 | -16.904 | -9.006 | 1.00 | 48.38 |
| | ATOM | 3906 | O | LEU | C | 693 | 19.382 | -16.426 | -9.402 | 1.00 | 46.35 |
| | ATOM | 3907 | N | LEU | C | 694 | 18.135 | -17.329 | -7.761 | 1.00 | 46.74 |
| 50 | ATOM | 3908 | CA | LEU | C | 694 | 19.204 | -17.272 | -6.775 | 1.00 | 49.41 |
| | ATOM | 3909 | CB | LEU | C | 694 | 18.634 | -17.415 | -5.362 | 1.00 | 45.20 |
| | ATOM | 3910 | CG | LEU | C | 694 | 18.222 | -16.128 | -4.643 | 1.00 | 40.19 |
| | ATOM | 3911 | CD1 | LEU | C | 694 | 17.456 | -16.474 | -3.371 | 1.00 | 41.65 |
| | ATOM | 3912 | CD2 | LEU | C | 694 | 19.453 | -15.307 | -4.317 | 1.00 | 35.91 |
| 55 | ATOM | 3913 | C | LEU | C | 694 | 20.172 | -18.417 | -7.058 | 1.00 | 54.15 |
| | ATOM | 3914 | O | LEU | C | 694 | 21.370 | -18.320 | -6.776 | 1.00 | 53.55 |
| | ATOM | 3915 | N | GLN | C | 695 | 19.634 | -19.498 | -7.619 | 1.00 | 57.44 |
| | ATOM | 3916 | CA | GLN | C | 695 | 20.416 | -20.685 | -7.959 | 1.00 | 62.46 |
| | ATOM | 3917 | CB | GLN | C | 695 | 19.477 | -21.853 | -8.304 | 1.00 | 61.95 |
| 60 | ATOM | 3918 | CG | GLN | C | 695 | 19.548 | -23.010 | -7.311 | 1.00 | 61.49 |
| | ATOM | 3919 | CD | GLN | C | 695 | 18.454 | -24.053 | -7.490 | 1.00 | 62.78 |

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|----|------|------|-----|-----|---|-----|---------|---------|---------|------|-------|
| 5 | ATOM | 3920 | OE1 | GLN | C | 695 | 18.262 | -24.928 | -6.653 | 1.00 | 63.33 |
| | ATOM | 3921 | NE2 | GLN | C | 695 | 17.720 | -23.969 | -8.608 | 1.00 | 60.37 |
| | ATOM | 3922 | C | GLN | C | 695 | 21.330 | -20.414 | -9.149 | 1.00 | 65.13 |
| | ATOM | 3923 | O | GLN | C | 695 | 22.517 | -20.740 | -9.116 | 1.00 | 65.87 |
| | ATOM | 3924 | N | ASP | C | 696 | 20.761 | -19.824 | -10.197 | 1.00 | 67.67 |
| 10 | ATOM | 3925 | CA | ASP | C | 696 | 21.492 | -19.500 | -11.420 | 1.00 | 70.66 |
| | ATOM | 3926 | CB | ASP | C | 696 | 20.801 | -18.348 | -12.151 | 1.00 | 71.06 |
| | ATOM | 3927 | CG | ASP | C | 696 | 20.127 | -18.792 | -13.430 | 1.00 | 71.70 |
| | ATOM | 3928 | OD1 | ASP | C | 696 | 20.637 | -18.455 | -14.521 | 1.00 | 72.47 |
| | ATOM | 3929 | OD2 | ASP | C | 696 | 19.086 | -19.478 | -13.342 | 1.00 | 71.41 |
| 15 | ATOM | 3930 | C | ASP | C | 696 | 22.951 | -19.132 | -11.169 | 1.00 | 72.41 |
| | ATOM | 3931 | O | ASP | C | 696 | 23.245 | -18.115 | -10.541 | 1.00 | 72.56 |
| | ATOM | 3932 | N | SER | C | 697 | 23.859 | -19.967 | -11.668 | 1.00 | 74.67 |
| | ATOM | 3933 | CA | SER | C | 697 | 25.291 | -19.741 | -11.507 | 1.00 | 76.45 |
| | ATOM | 3934 | CB | SER | C | 697 | 26.019 | -21.076 | -11.377 | 1.00 | 76.00 |
| 20 | ATOM | 3935 | C | SER | C | 697 | 25.841 | -18.960 | -12.696 | 1.00 | 78.44 |
| | ATOM | 3936 | O | SER | C | 697 | 26.286 | -17.809 | -12.489 | 1.00 | 79.20 |
| | ATOM | 3937 | OXT | SER | C | 697 | 25.818 | -19.510 | -13.820 | 1.00 | 80.07 |
| | ATOM | 3938 | CB | LYS | D | 686 | -14.070 | 13.661 | 16.843 | 1.00 | 50.28 |
| | ATOM | 3939 | C | LYS | D | 686 | -13.682 | 14.418 | 19.199 | 1.00 | 51.59 |
| 25 | ATOM | 3940 | O | LYS | D | 686 | -12.629 | 14.738 | 19.759 | 1.00 | 50.42 |
| | ATOM | 3941 | N | LYS | D | 686 | -12.910 | 15.796 | 17.283 | 1.00 | 50.43 |
| | ATOM | 3942 | CA | LYS | D | 686 | -13.976 | 14.872 | 17.769 | 1.00 | 50.62 |
| | ATOM | 3943 | N | HIS | D | 687 | -14.617 | 13.676 | 19.787 | 1.00 | 49.91 |
| | ATOM | 3944 | CA | HIS | D | 687 | -14.447 | 13.176 | 21.144 | 1.00 | 51.28 |
| 30 | ATOM | 3945 | CB | HIS | D | 687 | -15.806 | 12.984 | 21.828 | 1.00 | 54.12 |
| | ATOM | 3946 | CG | HIS | D | 687 | -15.713 | 12.336 | 23.177 | 1.00 | 60.06 |
| | ATOM | 3947 | CD2 | HIS | D | 687 | -15.418 | 11.064 | 23.539 | 1.00 | 61.05 |
| | ATOM | 3948 | ND1 | HIS | D | 687 | -15.911 | 13.030 | 24.352 | 1.00 | 62.39 |
| | ATOM | 3949 | CE1 | HIS | D | 687 | -15.741 | 12.215 | 25.378 | 1.00 | 62.76 |
| 35 | ATOM | 3950 | NE2 | HIS | D | 687 | -15.441 | 11.016 | 24.912 | 1.00 | 63.46 |
| | ATOM | 3951 | C | HIS | D | 687 | -13.691 | 11.849 | 21.163 | 1.00 | 49.55 |
| | ATOM | 3952 | O | HIS | D | 687 | -14.099 | 10.878 | 20.524 | 1.00 | 50.84 |
| | ATOM | 3953 | N | LYS | D | 688 | -12.593 | 11.816 | 21.909 | 1.00 | 44.00 |
| | ATOM | 3954 | CA | LYS | D | 688 | -11.784 | 10.611 | 22.038 | 1.00 | 40.31 |
| 40 | ATOM | 3955 | CB | LYS | D | 688 | -10.446 | 10.773 | 21.299 | 1.00 | 41.42 |
| | ATOM | 3956 | CG | LYS | D | 688 | -10.513 | 10.595 | 19.780 | 1.00 | 42.76 |
| | ATOM | 3957 | CD | LYS | D | 688 | -9.123 | 10.716 | 19.152 | 1.00 | 38.66 |
| | ATOM | 3958 | CE | LYS | D | 688 | -9.162 | 10.529 | 17.640 | 1.00 | 38.28 |
| | ATOM | 3959 | NZ | LYS | D | 688 | -7.894 | 10.970 | 16.986 | 1.00 | 31.58 |
| 45 | ATOM | 3960 | C | LYS | D | 688 | -11.506 | 10.378 | 23.517 | 1.00 | 36.70 |
| | ATOM | 3961 | O | LYS | D | 688 | -11.271 | 11.326 | 24.266 | 1.00 | 33.38 |
| | ATOM | 3962 | N | ILE | D | 689 | -11.549 | 9.122 | 23.942 | 1.00 | 33.06 |
| | ATOM | 3963 | CA | ILE | D | 689 | -11.255 | 8.806 | 25.328 | 1.00 | 28.70 |
| | ATOM | 3964 | CB | ILE | D | 689 | -11.438 | 7.301 | 25.607 | 1.00 | 30.88 |
| 50 | ATOM | 3965 | CG2 | ILE | D | 689 | -10.725 | 6.912 | 26.899 | 1.00 | 31.45 |
| | ATOM | 3966 | CG1 | ILE | D | 689 | -12.927 | 6.971 | 25.721 | 1.00 | 32.57 |
| | ATOM | 3967 | CD1 | ILE | D | 689 | -13.308 | 5.679 | 25.031 | 1.00 | 29.79 |
| | ATOM | 3968 | C | ILE | D | 689 | -9.790 | 9.193 | 25.541 | 1.00 | 27.64 |
| | ATOM | 3969 | O | ILE | D | 689 | -9.405 | 9.649 | 26.611 | 1.00 | 25.54 |
| 55 | ATOM | 3970 | N | LEU | D | 690 | -8.985 | 9.021 | 24.496 | 1.00 | 24.25 |
| | ATOM | 3971 | CA | LEU | D | 690 | -7.563 | 9.348 | 24.549 | 1.00 | 26.63 |
| | ATOM | 3972 | CB | LEU | D | 690 | -6.903 | 9.021 | 23.200 | 1.00 | 22.83 |
| | ATOM | 3973 | CG | LEU | D | 690 | -5.433 | 9.387 | 22.992 | 1.00 | 25.47 |
| | ATOM | 3974 | CD1 | LEU | D | 690 | -4.595 | 8.772 | 24.108 | 1.00 | 24.03 |
| 60 | ATOM | 3975 | CD2 | LEU | D | 690 | -4.956 | 8.898 | 21.616 | 1.00 | 20.87 |
| | ATOM | 3976 | C | LEU | D | 690 | -7.344 | 10.823 | 24.902 | 1.00 | 26.64 |

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|----|--------|------|-----|-----|---|-----|---------|--------|--------|------|-------|
| 5 | ATOM | 3977 | O | LEU | D | 690 | -6.408 | 11.165 | 25.625 | 1.00 | 28.34 |
| | ATOM | 3978 | N | HIS | D | 691 | -8.206 | 11.694 | 24.383 | 1.00 | 27.77 |
| | ATOM | 3979 | CA | HIS | D | 691 | -8.107 | 13.125 | 24.665 | 1.00 | 29.16 |
| | ATOM | 3980 | CB | HIS | D | 691 | -9.156 | 13.907 | 23.861 | 1.00 | 30.89 |
| 10 | ATOM | 3981 | CG | HIS | D | 691 | -8.903 | 13.935 | 22.386 | 1.00 | 37.09 |
| | ATOM | 3982 | CD2 | HIS | D | 691 | -7.750 | 14.000 | 21.679 | 1.00 | 41.39 |
| | ATOM | 3983 | ND1 | HIS | D | 691 | -9.920 | 13.906 | 21.458 | 1.00 | 41.65 |
| | ATOM | 3984 | CE1 | HIS | D | 691 | -9.407 | 13.953 | 20.242 | 1.00 | 44.64 |
| | ATOM | 3985 | NE2 | HIS | D | 691 | -8.091 | 14.010 | 20.347 | 1.00 | 41.94 |
| | ATOM | 3986 | C | HIS | D | 691 | -8.338 | 13.373 | 26.159 | 1.00 | 26.65 |
| 15 | ATOM | 3987 | O | HIS | D | 691 | -7.602 | 14.120 | 26.802 | 1.00 | 24.50 |
| | ATOM | 3988 | N | ARG | D | 692 | -9.371 | 12.742 | 26.703 | 1.00 | 25.70 |
| | ATOM | 3989 | CA | ARG | D | 692 | -9.691 | 12.912 | 28.114 | 1.00 | 29.11 |
| | ATOM | 3990 | CB | ARG | D | 692 | -10.959 | 12.134 | 28.472 | 1.00 | 30.84 |
| 20 | ATOM | 3991 | CG | ARG | D | 692 | -11.255 | 12.129 | 29.963 | 1.00 | 41.63 |
| | ATOM | 3992 | CD | ARG | D | 692 | -12.502 | 11.327 | 30.290 | 1.00 | 48.83 |
| | ATOM | 3993 | NE | ARG | D | 692 | -13.618 | 12.198 | 30.647 | 1.00 | 54.50 |
| | ATOM | 3994 | CZ | ARG | D | 692 | -14.498 | 12.677 | 29.774 | 1.00 | 59.37 |
| | ATOM | 3995 | NH1 | ARG | D | 692 | -14.392 | 12.371 | 28.486 | 1.00 | 60.97 |
| | ATOM | 3996 | NH2 | ARG | D | 692 | -15.483 | 13.464 | 30.188 | 1.00 | 59.07 |
| 25 | ATOM | 3997 | C | ARG | D | 692 | -8.548 | 12.451 | 29.011 | 1.00 | 28.30 |
| | ATOM | 3998 | O | ARG | D | 692 | -8.139 | 13.167 | 29.929 | 1.00 | 26.50 |
| | ATOM | 3999 | N | LEU | D | 693 | -8.030 | 11.259 | 28.737 | 1.00 | 24.87 |
| | ATOM | 4000 | CA | LEU | D | 693 | -6.943 | 10.705 | 29.536 | 1.00 | 27.17 |
| | ATOM | 4001 | CB | LEU | D | 693 | -6.674 | 9.254 | 29.116 | 1.00 | 28.45 |
| 30 | ATOM | 4002 | CG | LEU | D | 693 | -7.844 | 8.300 | 29.391 | 1.00 | 30.40 |
| | ATOM | 4003 | CD1 | LEU | D | 693 | -7.575 | 6.932 | 28.778 | 1.00 | 34.79 |
| | ATOM | 4004 | CD2 | LEU | D | 693 | -8.043 | 8.171 | 30.894 | 1.00 | 32.02 |
| | ATOM | 4005 | C | LEU | D | 693 | -5.670 | 11.539 | 29.440 | 1.00 | 25.96 |
| | ATOM | 4006 | O | LEU | D | 693 | -4.948 | 11.700 | 30.428 | 1.00 | 27.01 |
| 35 | ATOM | 4007 | N | LEU | D | 694 | -5.395 | 12.080 | 28.257 | 1.00 | 25.33 |
| | ATOM | 4008 | CA | LEU | D | 694 | -4.207 | 12.906 | 28.062 | 1.00 | 27.22 |
| | ATOM | 4009 | CB | LEU | D | 694 | -3.948 | 13.126 | 26.572 | 1.00 | 24.61 |
| | ATOM | 4010 | CG | LEU | D | 694 | -3.118 | 12.080 | 25.825 | 1.00 | 22.20 |
| | ATOM | 4011 | CD1 | LEU | D | 694 | -3.230 | 12.332 | 24.324 | 1.00 | 21.13 |
| 40 | ATOM | 4012 | CD2 | LEU | D | 694 | -1.666 | 12.148 | 26.275 | 1.00 | 21.34 |
| | ATOM | 4013 | C | LEU | D | 694 | -4.336 | 14.270 | 28.742 | 1.00 | 32.40 |
| | ATOM | 4014 | O | LEU | D | 694 | -3.339 | 14.889 | 29.102 | 1.00 | 31.55 |
| | ATOM | 4015 | N | GLN | D | 695 | -5.570 | 14.733 | 28.915 | 1.00 | 36.93 |
| | ATOM | 4016 | CA | GLN | D | 695 | -5.820 | 16.032 | 29.528 | 1.00 | 43.18 |
| 45 | ATOM | 4017 | CB | GLN | D | 695 | -7.022 | 16.694 | 28.862 | 1.00 | 40.48 |
| | ATOM | 4018 | CG | GLN | D | 695 | -6.772 | 17.071 | 27.422 | 1.00 | 37.99 |
| | ATOM | 4019 | CD | GLN | D | 695 | -7.943 | 17.764 | 26.795 | 1.00 | 35.86 |
| | ATOM | 4020 | OE1 | GLN | D | 695 | -7.863 | 18.895 | 26.342 | 1.00 | 38.84 |
| | ATOM | 4021 | NE2 | GLN | D | 695 | -9.082 | 17.060 | 26.757 | 1.00 | 31.62 |
| 50 | ATOM | 4022 | C | GLN | D | 695 | -6.049 | 16.009 | 31.034 | 1.00 | 48.74 |
| | ATOM | 4023 | O | GLN | D | 695 | -6.119 | 17.065 | 31.660 | 1.00 | 51.25 |
| | ATOM | 4024 | N | ASP | D | 696 | -6.175 | 14.818 | 31.611 | 1.00 | 54.01 |
| | ATOM | 4025 | CA | ASP | D | 696 | -6.398 | 14.702 | 33.047 | 1.00 | 62.23 |
| | ATOM | 4026 | CB | ASP | D | 696 | -6.217 | 13.238 | 33.485 | 1.00 | 63.97 |
| 55 | ATOM | 4027 | CG | ASP | D | 696 | -7.527 | 12.467 | 33.475 | 1.00 | 67.72 |
| | ATOM | 4028 | OD1 | ASP | D | 696 | -8.528 | 12.996 | 32.941 | 1.00 | 68.11 |
| | ATOM | 4029 | OD2 | ASP | D | 696 | -7.552 | 11.333 | 34.003 | 1.00 | 68.95 |
| | ATOM | 4030 | C | ASP | D | 696 | -5.456 | 15.622 | 33.840 | 1.00 | 65.60 |
| | ATOM | 4031 | O | ASP | D | 696 | -4.312 | 15.189 | 34.134 | 1.00 | 68.33 |
| 60 | ATOM | 4032 | OXT | ASP | D | 696 | -5.874 | 16.755 | 34.140 | 1.00 | 69.20 |
| | HETATM | 4033 | O | HOH | | 1 | 16.153 | -0.605 | -4.425 | 1.00 | 17.11 |

| | | | | | | | | | | |
|----|--------|------|---|-----|----|--------|---------|---------|------|-------|
| 5 | HETATM | 4034 | O | HOH | 2 | 16.570 | -5.304 | -16.560 | 1.00 | 21.44 |
| | HETATM | 4035 | O | HOH | 3 | 18.526 | 0.742 | -4.495 | 1.00 | 23.43 |
| | HETATM | 4036 | O | HOH | 4 | 13.647 | -2.187 | 8.588 | 1.00 | 25.82 |
| | HETATM | 4037 | O | HOH | 5 | 9.778 | -5.825 | 2.509 | 1.00 | 20.58 |
| | HETATM | 4038 | O | HOH | 6 | 17.072 | -3.605 | -8.015 | 1.00 | 18.38 |
| 10 | HETATM | 4039 | O | HOH | 7 | 24.920 | -1.689 | -2.780 | 1.00 | 25.74 |
| | HETATM | 4040 | O | HOH | 8 | 7.321 | -5.649 | 5.061 | 1.00 | 24.11 |
| | HETATM | 4041 | O | HOH | 9 | 25.976 | -3.535 | 15.158 | 1.00 | 26.78 |
| | HETATM | 4042 | O | HOH | 10 | 15.088 | -7.006 | -15.192 | 1.00 | 19.64 |
| | HETATM | 4043 | O | HOH | 11 | 14.070 | 0.925 | -5.953 | 1.00 | 20.55 |
| 15 | HETATM | 4044 | O | HOH | 12 | 18.008 | 3.407 | -6.654 | 1.00 | 32.30 |
| | HETATM | 4045 | O | HOH | 13 | 31.949 | -8.393 | 13.487 | 1.00 | 30.64 |
| | HETATM | 4046 | O | HOH | 14 | 19.625 | -2.804 | -4.279 | 1.00 | 24.45 |
| | HETATM | 4047 | O | HOH | 15 | 11.741 | 1.079 | -21.140 | 1.00 | 25.87 |
| | HETATM | 4048 | O | HOH | 16 | 25.067 | 13.951 | 14.153 | 1.00 | 31.07 |
| 20 | HETATM | 4049 | O | HOH | 17 | 15.501 | 1.323 | -10.393 | 1.00 | 21.01 |
| | HETATM | 4050 | O | HOH | 18 | 13.880 | 3.349 | -11.482 | 1.00 | 24.28 |
| | HETATM | 4051 | O | HOH | 19 | 17.591 | 0.979 | -8.828 | 1.00 | 35.26 |
| | HETATM | 4052 | O | HOH | 20 | 23.682 | -2.041 | -0.314 | 1.00 | 37.90 |
| | HETATM | 4053 | O | HOH | 21 | 15.754 | 9.496 | 11.841 | 1.00 | 39.44 |
| 25 | HETATM | 4054 | O | HOH | 22 | -4.943 | 7.574 | -3.066 | 1.00 | 37.67 |
| | HETATM | 4055 | O | HOH | 23 | 6.877 | 0.354 | -15.982 | 1.00 | 36.92 |
| | HETATM | 4056 | O | HOH | 24 | 15.806 | -4.002 | 8.671 | 1.00 | 30.38 |
| | HETATM | 4057 | O | HOH | 25 | 17.185 | -3.158 | -5.321 | 1.00 | 28.89 |
| | HETATM | 4058 | O | HOH | 26 | 17.572 | 9.249 | 17.009 | 1.00 | 30.15 |
| 30 | HETATM | 4059 | O | HOH | 27 | 24.096 | -2.929 | 11.604 | 1.00 | 31.37 |
| | HETATM | 4060 | O | HOH | 28 | 22.324 | -5.871 | -11.980 | 1.00 | 32.74 |
| | HETATM | 4061 | O | HOH | 29 | 27.547 | -12.361 | -0.801 | 1.00 | 36.61 |
| | HETATM | 4062 | O | HOH | 30 | 11.173 | 13.442 | -2.719 | 1.00 | 35.41 |
| | HETATM | 4063 | O | HOH | 31 | 15.438 | -9.527 | 5.483 | 1.00 | 29.88 |
| 35 | HETATM | 4064 | O | HOH | 32 | 9.946 | -6.564 | 5.983 | 1.00 | 35.05 |
| | HETATM | 4065 | O | HOH | 33 | 7.599 | 11.680 | -15.261 | 1.00 | 38.68 |
| | HETATM | 4066 | O | HOH | 34 | 20.112 | 10.503 | -5.109 | 1.00 | 42.66 |
| | HETATM | 4067 | O | HOH | 35 | 15.972 | 10.343 | 14.897 | 1.00 | 41.73 |
| | HETATM | 4068 | O | HOH | 36 | 22.401 | -5.914 | -9.527 | 1.00 | 28.08 |
| 40 | HETATM | 4069 | O | HOH | 37 | 16.128 | -0.899 | -8.109 | 1.00 | 33.13 |
| | HETATM | 4070 | O | HOH | 38 | 3.581 | 15.655 | -3.706 | 1.00 | 41.37 |
| | HETATM | 4071 | O | HOH | 39 | 31.900 | 13.545 | 21.339 | 1.00 | 37.79 |
| | HETATM | 4072 | O | HOH | 40 | 20.058 | -7.530 | 14.119 | 1.00 | 47.51 |
| | HETATM | 4073 | O | HOH | 41 | 34.634 | 6.668 | 15.632 | 1.00 | 29.24 |
| 45 | HETATM | 4074 | O | HOH | 42 | 17.968 | 10.511 | -9.085 | 1.00 | 44.60 |
| | HETATM | 4075 | O | HOH | 43 | 23.258 | -17.325 | -4.088 | 1.00 | 44.10 |
| | HETATM | 4076 | O | HOH | 44 | 4.034 | -1.472 | 27.521 | 1.00 | 15.22 |
| | HETATM | 4077 | O | HOH | 45 | -5.943 | -0.018 | 36.088 | 1.00 | 21.11 |
| | HETATM | 4078 | O | HOH | 46 | 6.084 | -1.509 | 29.478 | 1.00 | 19.51 |
| 50 | HETATM | 4079 | O | HOH | 47 | 9.762 | 1.061 | 15.621 | 1.00 | 27.74 |
| | HETATM | 4080 | O | HOH | 48 | 1.804 | 0.717 | 17.260 | 1.00 | 20.97 |
| | HETATM | 4081 | O | HOH | 49 | 0.929 | 0.421 | 30.281 | 1.00 | 19.64 |
| | HETATM | 4082 | O | HOH | 50 | 9.627 | 4.271 | 31.231 | 1.00 | 19.02 |
| | HETATM | 4083 | O | HOH | 51 | 2.121 | -0.261 | 13.654 | 1.00 | 26.09 |
| 55 | HETATM | 4084 | O | HOH | 52 | 20.060 | 10.275 | 17.711 | 1.00 | 25.49 |
| | HETATM | 4085 | O | HOH | 53 | -6.786 | 0.736 | 33.483 | 1.00 | 22.34 |
| | HETATM | 4086 | O | HOH | 54 | 2.751 | -4.136 | 27.760 | 1.00 | 19.93 |
| | HETATM | 4087 | O | HOH | 55 | 5.994 | -4.079 | 31.292 | 1.00 | 32.27 |
| | HETATM | 4088 | O | HOH | 56 | 19.416 | 16.921 | 21.645 | 1.00 | 25.54 |
| 60 | HETATM | 4089 | O | HOH | 57 | 4.833 | 2.325 | 29.006 | 1.00 | 19.00 |
| | HETATM | 4090 | O | HOH | 58 | -7.638 | -8.931 | 37.809 | 1.00 | 24.79 |

| | | | | | | | | | | |
|----|--------|------|---|-----|-----|---------|---------|---------|------|-------|
| 5 | HETATM | 4091 | O | HOH | 59 | 28.442 | -4.673 | 21.875 | 1.00 | 24.32 |
| | HETATM | 4092 | O | HOH | 60 | 1.094 | -4.893 | 32.100 | 1.00 | 24.27 |
| | HETATM | 4093 | O | HOH | 61 | 0.905 | -7.306 | 32.783 | 1.00 | 21.33 |
| | HETATM | 4094 | O | HOH | 62 | 3.396 | -2.971 | 32.306 | 1.00 | 26.13 |
| | HETATM | 4095 | O | HOH | 63 | 10.363 | 4.576 | 28.391 | 1.00 | 33.43 |
| 10 | HETATM | 4096 | O | HOH | 64 | 19.551 | -6.473 | 16.597 | 1.00 | 35.38 |
| | HETATM | 4097 | O | HOH | 65 | -2.888 | -19.627 | 15.665 | 1.00 | 27.99 |
| | HETATM | 4098 | O | HOH | 66 | -7.275 | -9.745 | 31.077 | 1.00 | 27.00 |
| | HETATM | 4099 | O | HOH | 67 | 10.189 | 3.580 | 16.510 | 1.00 | 24.19 |
| | HETATM | 4100 | O | HOH | 68 | 2.741 | 0.716 | 28.382 | 1.00 | 16.48 |
| 15 | HETATM | 4101 | O | HOH | 69 | 23.522 | -4.323 | 13.943 | 1.00 | 27.48 |
| | HETATM | 4102 | O | HOH | 70 | 17.133 | 8.133 | 19.686 | 1.00 | 32.24 |
| | HETATM | 4103 | O | HOH | 71 | -0.295 | 4.535 | 35.884 | 1.00 | 33.42 |
| | HETATM | 4104 | O | HOH | 72 | 9.519 | 10.828 | 34.842 | 1.00 | 29.38 |
| | HETATM | 4105 | O | HOH | 73 | 6.291 | 14.878 | 29.070 | 1.00 | 28.21 |
| 20 | HETATM | 4106 | O | HOH | 74 | -1.721 | 6.480 | 13.381 | 1.00 | 49.91 |
| | HETATM | 4107 | O | HOH | 75 | 10.091 | -15.427 | 26.194 | 1.00 | 24.17 |
| | HETATM | 4108 | O | HOH | 76 | 5.029 | 7.461 | 17.718 | 1.00 | 18.91 |
| | HETATM | 4109 | O | HOH | 77 | 3.758 | 2.086 | 14.306 | 1.00 | 28.28 |
| | HETATM | 4110 | O | HOH | 78 | -1.390 | -18.739 | 33.183 | 1.00 | 41.11 |
| 25 | HETATM | 4111 | O | HOH | 79 | 12.703 | -8.687 | 32.119 | 1.00 | 36.21 |
| | HETATM | 4112 | O | HOH | 80 | 22.270 | -6.451 | 14.844 | 1.00 | 33.21 |
| | HETATM | 4113 | O | HOH | 81 | 1.458 | 4.605 | 34.026 | 1.00 | 23.59 |
| | HETATM | 4114 | O | HOH | 82 | 1.759 | -2.158 | 30.374 | 1.00 | 28.78 |
| | HETATM | 4115 | O | HOH | 83 | 6.153 | -21.372 | 23.188 | 1.00 | 31.14 |
| 30 | HETATM | 4116 | O | HOH | 84 | 36.525 | 0.463 | 20.792 | 1.00 | 45.26 |
| | HETATM | 4117 | O | HOH | 85 | 13.832 | 9.696 | 13.792 | 1.00 | 33.12 |
| | HETATM | 4118 | O | HOH | 86 | 31.166 | 6.635 | 24.924 | 1.00 | 35.19 |
| | HETATM | 4119 | O | HOH | 87 | 8.844 | -10.389 | 34.180 | 1.00 | 48.80 |
| | HETATM | 4120 | O | HOH | 88 | 9.581 | -6.956 | 34.136 | 1.00 | 42.95 |
| 35 | HETATM | 4121 | O | HOH | 89 | -1.563 | 15.887 | 27.596 | 1.00 | 39.35 |
| | HETATM | 4122 | O | HOH | 90 | -5.286 | 10.345 | 32.757 | 1.00 | 35.20 |
| | HETATM | 4123 | O | HOH | 91 | 15.035 | 0.607 | 13.339 | 1.00 | 29.53 |
| | HETATM | 4124 | O | HOH | 92 | -10.984 | -1.500 | 30.272 | 1.00 | 29.84 |
| | HETATM | 4125 | O | HOH | 93 | -7.239 | -0.271 | -1.207 | 1.00 | 48.98 |
| 40 | HETATM | 4126 | O | HOH | 94 | 18.022 | -4.902 | 34.286 | 1.00 | 35.28 |
| | HETATM | 4127 | O | HOH | 95 | 29.347 | -6.319 | 19.920 | 1.00 | 37.20 |
| | HETATM | 4128 | O | HOH | 96 | -14.309 | -19.369 | 20.945 | 1.00 | 30.23 |
| | HETATM | 4129 | O | HOH | 97 | 31.496 | 4.614 | 18.716 | 1.00 | 38.79 |
| | HETATM | 4130 | O | HOH | 98 | 26.567 | 9.759 | 25.629 | 1.00 | 29.72 |
| 45 | HETATM | 4131 | O | HOH | 99 | 2.848 | 14.531 | 1.134 | 1.00 | 38.08 |
| | HETATM | 4132 | O | HOH | 100 | -9.373 | 5.699 | -7.953 | 1.00 | 53.23 |
| | HETATM | 4133 | O | HOH | 101 | -10.137 | -0.553 | -6.742 | 1.00 | 47.72 |
| | HETATM | 4134 | O | HOH | 102 | 10.558 | -10.363 | 15.403 | 1.00 | 40.97 |
| | HETATM | 4135 | O | HOH | 103 | 21.079 | 17.166 | 18.929 | 1.00 | 32.40 |
| 50 | HETATM | 4136 | O | HOH | 104 | 25.810 | -5.921 | 22.506 | 1.00 | 37.69 |
| | HETATM | 4137 | O | HOH | 105 | 22.493 | -1.311 | 34.465 | 1.00 | 49.94 |
| | HETATM | 4138 | O | HOH | 106 | 19.317 | 10.977 | 38.703 | 1.00 | 40.60 |
| | HETATM | 4139 | O | HOH | 107 | 4.479 | 13.951 | 3.045 | 1.00 | 45.33 |
| | HETATM | 4140 | O | HOH | 108 | 20.418 | 19.353 | 34.044 | 1.00 | 42.18 |
| 55 | HETATM | 4141 | O | HOH | 109 | -3.065 | 8.936 | 14.062 | 1.00 | 38.41 |
| | HETATM | 4142 | O | HOH | 110 | 26.856 | -4.674 | -10.940 | 1.00 | 55.67 |
| | HETATM | 4143 | O | HOH | 111 | 2.032 | -6.387 | 5.614 | 1.00 | 42.23 |
| | HETATM | 4144 | O | HOH | 112 | 0.601 | 0.228 | -17.268 | 1.00 | 40.57 |
| | HETATM | 4145 | O | HOH | 113 | 4.903 | 13.488 | -14.050 | 1.00 | 47.72 |
| 60 | HETATM | 4146 | O | HOH | 114 | 3.986 | 16.140 | -0.960 | 1.00 | 40.66 |
| | HETATM | 4147 | O | HOH | 115 | 12.968 | -19.561 | 2.741 | 1.00 | 40.76 |

| | | | | | | | | | | |
|----|--------|------|---|-----|-----|---------|---------|---------|------|-------|
| 5 | HETATM | 4148 | O | HOH | 116 | 7.170 | 15.583 | 2.599 | 1.00 | 43.69 |
| | HETATM | 4149 | O | HOH | 117 | -1.966 | 10.606 | 3.572 | 1.00 | 52.63 |
| | HETATM | 4150 | O | HOH | 118 | 29.030 | 10.644 | 6.707 | 1.00 | 42.54 |
| | HETATM | 4151 | O | HOH | 119 | 0.468 | 4.354 | 8.374 | 1.00 | 38.69 |
| | HETATM | 4152 | O | HOH | 120 | 29.086 | 17.119 | 19.272 | 1.00 | 45.51 |
| 10 | HETATM | 4153 | O | HOH | 121 | 24.614 | 17.609 | 20.174 | 1.00 | 53.55 |
| | HETATM | 4154 | O | HOH | 122 | -15.318 | 0.362 | 26.686 | 1.00 | 36.77 |
| | HETATM | 4155 | O | HOH | 123 | -3.857 | -24.786 | 28.325 | 1.00 | 39.64 |
| | HETATM | 4156 | O | HOH | 124 | 21.728 | 22.178 | 31.983 | 1.00 | 43.73 |
| | HETATM | 4157 | O | HOH | 125 | 31.650 | -7.370 | 21.642 | 1.00 | 40.53 |
| 15 | HETATM | 4158 | O | HOH | 126 | 25.421 | 10.436 | 21.161 | 1.00 | 32.31 |
| | HETATM | 4159 | O | HOH | 127 | 10.317 | -9.457 | 12.998 | 1.00 | 37.77 |
| | HETATM | 4160 | O | HOH | 128 | 22.723 | 14.887 | 15.427 | 1.00 | 47.90 |
| | HETATM | 4161 | O | HOH | 129 | 6.702 | 9.556 | 37.596 | 1.00 | 47.81 |
| | HETATM | 4162 | O | HOH | 130 | 27.987 | 13.557 | 7.167 | 1.00 | 41.15 |
| 20 | HETATM | 4163 | O | HOH | 131 | 30.798 | 16.499 | 7.588 | 1.00 | 58.47 |
| | HETATM | 4164 | O | HOH | 132 | 10.071 | -0.571 | -20.393 | 1.00 | 38.79 |
| | HETATM | 4165 | O | HOH | 133 | 9.562 | 8.334 | -21.392 | 1.00 | 36.80 |
| | HETATM | 4166 | O | HOH | 134 | 6.712 | 6.058 | 8.822 | 1.00 | 37.43 |
| | HETATM | 4167 | O | HOH | 135 | 5.927 | 8.454 | 10.594 | 1.00 | 42.34 |
| 25 | HETATM | 4168 | O | HOH | 136 | 4.472 | 6.306 | 10.973 | 1.00 | 37.35 |
| | HETATM | 4169 | O | HOH | 137 | 6.792 | 7.721 | 7.051 | 1.00 | 47.23 |
| | HETATM | 4170 | O | HOH | 138 | 24.513 | 11.582 | 33.724 | 1.00 | 45.55 |
| | HETATM | 4171 | O | HOH | 139 | -2.528 | -20.361 | 12.354 | 1.00 | 52.13 |
| | HETATM | 4172 | O | HOH | 140 | -7.864 | 7.706 | 19.248 | 1.00 | 47.82 |
| 30 | HETATM | 4173 | O | HOH | 141 | 11.577 | -16.962 | 24.398 | 1.00 | 39.43 |
| | HETATM | 4174 | O | HOH | 142 | 18.087 | 12.263 | -5.507 | 1.00 | 33.36 |
| | HETATM | 4175 | O | HOH | 143 | -6.816 | -14.190 | 10.674 | 1.00 | 51.32 |
| | HETATM | 4176 | O | HOH | 144 | -7.377 | -16.701 | 33.528 | 1.00 | 57.11 |
| | HETATM | 4177 | O | HOH | 145 | -5.379 | -20.107 | 32.689 | 1.00 | 43.01 |
| 35 | HETATM | 4178 | O | HOH | 146 | 8.766 | -7.947 | -16.274 | 1.00 | 49.96 |
| | HETATM | 4179 | O | HOH | 147 | 10.946 | -7.937 | -18.142 | 1.00 | 55.67 |

END

5

Appendix 3

Atomic Coordinates for Human ER α Complexed With OHT

| | | | | | | | | | | | | |
|----|--------|----------|----------|----------|----------|--------|--------|--------|------|-------|---|----|
| 10 | CRYST1 | 58.242 | 58.242 | 277.467 | 90.00 | 90.00 | 120.00 | P | 65 | 2 | 2 | 12 |
| | ORIGX1 | 1.000000 | 0.000000 | 0.000000 | 0.000000 | | | | | | | |
| | ORIGX2 | 0.000000 | 1.000000 | 0.000000 | 0.000000 | | | | | | | |
| | ORIGX3 | 0.000000 | 0.000000 | 1.000000 | 0.000000 | | | | | | | |
| | SCALE1 | 0.017170 | 0.009913 | 0.000000 | 0.000000 | | | | | | | |
| 15 | SCALE2 | 0.000000 | 0.019826 | 0.000000 | 0.000000 | | | | | | | |
| | SCALE3 | 0.000000 | 0.000000 | 0.003604 | 0.000000 | | | | | | | |
| | ATOM | 1 | CB | LEU | 306 | 6.638 | 11.502 | 3.989 | 1.00 | 61.20 | | |
| | ATOM | 2 | C | LEU | 306 | 7.381 | 10.684 | 6.231 | 1.00 | 61.47 | | |
| 20 | ATOM | 3 | O | LEU | 306 | 6.407 | 11.020 | 6.905 | 1.00 | 62.09 | | |
| | ATOM | 4 | N | LEU | 306 | 6.369 | 9.128 | 4.588 | 1.00 | 62.32 | | |
| | ATOM | 5 | CA | LEU | 306 | 7.232 | 10.330 | 4.754 | 1.00 | 61.30 | | |
| | ATOM | 6 | N | ALA | 307 | 8.609 | 10.605 | 6.730 | 1.00 | 60.52 | | |
| | ATOM | 7 | CA | ALA | 307 | 8.891 | 10.912 | 8.125 | 1.00 | 58.77 | | |
| 25 | ATOM | 8 | CB | ALA | 307 | 10.318 | 10.501 | 8.465 | 1.00 | 59.70 | | |
| | ATOM | 9 | C | ALA | 307 | 8.692 | 12.393 | 8.429 | 1.00 | 57.51 | | |
| | ATOM | 10 | O | ALA | 307 | 8.451 | 12.770 | 9.574 | 1.00 | 57.64 | | |
| | ATOM | 11 | N | LEU | 308 | 8.789 | 13.228 | 7.400 | 1.00 | 55.82 | | |
| | ATOM | 12 | CA | LEU | 308 | 8.638 | 14.668 | 7.573 | 1.00 | 56.62 | | |
| 30 | ATOM | 13 | CB | LEU | 308 | 9.298 | 15.402 | 6.406 | 1.00 | 57.48 | | |
| | ATOM | 14 | CG | LEU | 308 | 10.637 | 14.822 | 5.948 | 1.00 | 59.17 | | |
| | ATOM | 15 | CD1 | LEU | 308 | 10.474 | 14.189 | 4.569 | 1.00 | 60.38 | | |
| | ATOM | 16 | CD2 | LEU | 308 | 11.694 | 15.920 | 5.933 | 1.00 | 58.46 | | |
| | ATOM | 17 | C | LEU | 308 | 7.190 | 15.130 | 7.710 | 1.00 | 56.51 | | |
| 35 | ATOM | 18 | O | LEU | 308 | 6.935 | 16.307 | 7.961 | 1.00 | 55.58 | | |
| | ATOM | 19 | N | SER | 309 | 6.246 | 14.208 | 7.546 | 1.00 | 57.04 | | |
| | ATOM | 20 | CA | SER | 309 | 4.828 | 14.544 | 7.657 | 1.00 | 56.46 | | |
| | ATOM | 21 | CB | SER | 309 | 4.034 | 13.896 | 6.514 | 1.00 | 56.79 | | |
| | ATOM | 22 | OG | SER | 309 | 4.071 | 12.479 | 6.588 | 1.00 | 57.23 | | |
| 40 | ATOM | 23 | C | SER | 309 | 4.261 | 14.095 | 9.003 | 1.00 | 56.13 | | |
| | ATOM | 24 | O | SER | 309 | 3.166 | 14.507 | 9.398 | 1.00 | 55.17 | | |
| | ATOM | 25 | N | LEU | 310 | 5.016 | 13.257 | 9.706 | 1.00 | 54.31 | | |
| | ATOM | 26 | CA | LEU | 310 | 4.591 | 12.749 | 11.004 | 1.00 | 53.55 | | |
| | ATOM | 27 | CB | LEU | 310 | 5.651 | 11.811 | 11.582 | 1.00 | 54.40 | | |
| 45 | ATOM | 28 | CG | LEU | 310 | 5.586 | 10.333 | 11.189 | 1.00 | 56.49 | | |
| | ATOM | 29 | CD1 | LEU | 310 | 5.530 | 10.200 | 9.676 | 1.00 | 57.06 | | |
| | ATOM | 30 | CD2 | LEU | 310 | 6.809 | 9.610 | 11.739 | 1.00 | 57.28 | | |
| | ATOM | 31 | C | LEU | 310 | 4.330 | 13.865 | 12.003 | 1.00 | 53.18 | | |
| | ATOM | 32 | O | LEU | 310 | 4.993 | 14.905 | 11.984 | 1.00 | 53.17 | | |
| 50 | ATOM | 33 | N | THR | 311 | 3.352 | 13.641 | 12.874 | 1.00 | 51.71 | | |
| | ATOM | 34 | CA | THR | 311 | 3.017 | 14.604 | 13.912 | 1.00 | 49.93 | | |
| | ATOM | 35 | CB | THR | 311 | 1.527 | 14.554 | 14.275 | 1.00 | 48.96 | | |
| | ATOM | 36 | OG1 | THR | 311 | 1.242 | 13.311 | 14.930 | 1.00 | 47.20 | | |
| | ATOM | 37 | CG2 | THR | 311 | 0.666 | 14.688 | 13.027 | 1.00 | 50.99 | | |
| 55 | ATOM | 38 | C | THR | 311 | 3.815 | 14.201 | 15.145 | 1.00 | 48.84 | | |
| | ATOM | 39 | O | THR | 311 | 4.371 | 13.103 | 15.197 | 1.00 | 46.66 | | |
| | ATOM | 40 | N | ALA | 312 | 3.857 | 15.078 | 16.141 | 1.00 | 48.76 | | |
| | ATOM | 41 | CA | ALA | 312 | 4.590 | 14.798 | 17.369 | 1.00 | 47.75 | | |
| | ATOM | 42 | CB | ALA | 312 | 4.359 | 15.910 | 18.378 | 1.00 | 47.06 | | |
| 60 | ATOM | 43 | C | ALA | 312 | 4.171 | 13.460 | 17.964 | 1.00 | 47.41 | | |

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|----|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 44 | O | ALA | 312 | 5.009 | 12.609 | 18.262 | 1.00 | 45.52 |
| | ATOM | 45 | N | ASP | 313 | 2.868 | 13.275 | 18.143 | 1.00 | 47.58 |
| | ATOM | 46 | CA | ASP | 313 | 2.367 | 12.032 | 18.714 | 1.00 | 47.63 |
| | ATOM | 47 | CB | ASP | 313 | 0.848 | 12.100 | 18.879 | 1.00 | 51.96 |
| | ATOM | 48 | CG | ASP | 313 | 0.430 | 12.872 | 20.118 | 1.00 | 56.21 |
| 10 | ATOM | 49 | OD1 | ASP | 313 | 1.314 | 13.234 | 20.929 | 1.00 | 56.38 |
| | ATOM | 50 | OD2 | ASP | 313 | -0.785 | 13.117 | 20.282 | 1.00 | 59.15 |
| | ATOM | 51 | C | ASP | 313 | 2.745 | 10.846 | 17.835 | 1.00 | 43.93 |
| | ATOM | 52 | O | ASP | 313 | 2.959 | 9.741 | 18.330 | 1.00 | 44.77 |
| | ATOM | 53 | N | GLN | 314 | 2.826 | 11.081 | 16.531 | 1.00 | 44.52 |
| 15 | ATOM | 54 | CA | GLN | 314 | 3.182 | 10.028 | 15.588 | 1.00 | 44.73 |
| | ATOM | 55 | CB | GLN | 314 | 2.849 | 10.464 | 14.156 | 1.00 | 45.05 |
| | ATOM | 56 | CG | GLN | 314 | 1.534 | 9.886 | 13.626 | 1.00 | 48.47 |
| | ATOM | 57 | CD | GLN | 314 | 0.982 | 10.646 | 12.428 | 1.00 | 50.37 |
| | ATOM | 58 | OE1 | GLN | 314 | 1.649 | 11.515 | 11.856 | 1.00 | 49.38 |
| 20 | ATOM | 59 | NE2 | GLN | 314 | -0.248 | 10.318 | 12.043 | 1.00 | 51.74 |
| | ATOM | 60 | C | GLN | 314 | 4.673 | 9.722 | 15.707 | 1.00 | 43.26 |
| | ATOM | 61 | O | GLN | 314 | 5.100 | 8.580 | 15.555 | 1.00 | 43.93 |
| | ATOM | 62 | N | MET | 315 | 5.459 | 10.757 | 15.980 | 1.00 | 42.29 |
| | ATOM | 63 | CA | MET | 315 | 6.901 | 10.606 | 16.130 | 1.00 | 41.26 |
| 25 | ATOM | 64 | CB | MET | 315 | 7.565 | 11.985 | 16.224 | 1.00 | 42.43 |
| | ATOM | 65 | CG | MET | 315 | 9.082 | 11.939 | 16.356 | 1.00 | 42.34 |
| | ATOM | 66 | SD | MET | 315 | 9.906 | 11.190 | 14.925 | 1.00 | 46.22 |
| | ATOM | 67 | CE | MET | 315 | 9.547 | 12.408 | 13.680 | 1.00 | 37.32 |
| | ATOM | 68 | C | MET | 315 | 7.218 | 9.791 | 17.379 | 1.00 | 38.89 |
| 30 | ATOM | 69 | O | MET | 315 | 8.002 | 8.841 | 17.335 | 1.00 | 40.02 |
| | ATOM | 70 | N | VAL | 316 | 6.599 | 10.165 | 18.491 | 1.00 | 37.65 |
| | ATOM | 71 | CA | VAL | 316 | 6.819 | 9.476 | 19.756 | 1.00 | 39.56 |
| | ATOM | 72 | CB | VAL | 316 | 6.023 | 10.136 | 20.897 | 1.00 | 39.22 |
| | ATOM | 73 | CG1 | VAL | 316 | 6.245 | 9.373 | 22.192 | 1.00 | 44.43 |
| 35 | ATOM | 74 | CG2 | VAL | 316 | 6.446 | 11.583 | 21.059 | 1.00 | 41.04 |
| | ATOM | 75 | C | VAL | 316 | 6.404 | 8.012 | 19.664 | 1.00 | 40.04 |
| | ATOM | 76 | O | VAL | 316 | 7.141 | 7.117 | 20.077 | 1.00 | 37.86 |
| | ATOM | 77 | N | SER | 317 | 5.215 | 7.767 | 19.127 | 1.00 | 41.90 |
| | ATOM | 78 | CA | SER | 317 | 4.733 | 6.400 | 18.997 | 1.00 | 41.68 |
| 40 | ATOM | 79 | CB | SER | 317 | 3.311 | 6.402 | 18.415 | 1.00 | 43.85 |
| | ATOM | 80 | OG | SER | 317 | 3.225 | 5.631 | 17.230 | 1.00 | 49.38 |
| | ATOM | 81 | C | SER | 317 | 5.696 | 5.601 | 18.114 | 1.00 | 39.72 |
| | ATOM | 82 | O | SER | 317 | 6.011 | 4.446 | 18.407 | 1.00 | 40.21 |
| | ATOM | 83 | N | ALA | 318 | 6.182 | 6.220 | 17.043 | 1.00 | 38.35 |
| 45 | ATOM | 84 | CA | ALA | 318 | 7.114 | 5.540 | 16.153 | 1.00 | 36.96 |
| | ATOM | 85 | CB | ALA | 318 | 7.485 | 6.448 | 14.986 | 1.00 | 37.92 |
| | ATOM | 86 | C | ALA | 318 | 8.375 | 5.137 | 16.920 | 1.00 | 38.31 |
| | ATOM | 87 | O | ALA | 318 | 8.820 | 3.992 | 16.844 | 1.00 | 33.94 |
| | ATOM | 88 | N | LEU | 319 | 8.938 | 6.089 | 17.664 | 1.00 | 36.92 |
| 50 | ATOM | 89 | CA | LEU | 319 | 10.161 | 5.854 | 18.438 | 1.00 | 38.56 |
| | ATOM | 90 | CB | LEU | 319 | 10.660 | 7.174 | 19.040 | 1.00 | 40.86 |
| | ATOM | 91 | CG | LEU | 319 | 11.136 | 8.264 | 18.071 | 1.00 | 41.25 |
| | ATOM | 92 | CD1 | LEU | 319 | 11.714 | 9.440 | 18.857 | 1.00 | 44.30 |
| | ATOM | 93 | CD2 | LEU | 319 | 12.182 | 7.693 | 17.140 | 1.00 | 42.61 |
| 55 | ATOM | 94 | C | LEU | 319 | 9.965 | 4.826 | 19.549 | 1.00 | 38.33 |
| | ATOM | 95 | O | LEU | 319 | 10.779 | 3.916 | 19.729 | 1.00 | 33.91 |
| | ATOM | 96 | N | LEU | 320 | 8.879 | 4.982 | 20.297 | 1.00 | 37.39 |
| | ATOM | 97 | CA | LEU | 320 | 8.567 | 4.067 | 21.387 | 1.00 | 41.55 |
| | ATOM | 98 | CB | LEU | 320 | 7.239 | 4.467 | 22.049 | 1.00 | 38.47 |
| 60 | ATOM | 99 | CG | LEU | 320 | 7.236 | 5.582 | 23.099 | 1.00 | 44.81 |
| | ATOM | 100 | CD1 | LEU | 320 | 5.876 | 5.634 | 23.802 | 1.00 | 44.96 |

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|----|------|-----|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 101 | CD2 | LEU | 320 | 8.334 | 5.332 | 24.112 | 1.00 | 43.36 |
| | ATOM | 102 | C | LEU | 320 | 8.466 | 2.642 | 20.843 | 1.00 | 41.11 |
| | ATOM | 103 | O | LEU | 320 | 8.971 | 1.697 | 21.443 | 1.00 | 41.87 |
| | ATOM | 104 | N | ASP | 321 | 7.812 | 2.504 | 19.696 | 1.00 | 43.94 |
| | ATOM | 105 | CA | ASP | 321 | 7.613 | 1.210 | 19.053 | 1.00 | 44.77 |
| 10 | ATOM | 106 | CB | ASP | 321 | 6.669 | 1.372 | 17.860 | 1.00 | 48.39 |
| | ATOM | 107 | CG | ASP | 321 | 5.206 | 1.318 | 18.255 | 1.00 | 52.39 |
| | ATOM | 108 | OD1 | ASP | 321 | 4.901 | 1.422 | 19.464 | 1.00 | 53.56 |
| | ATOM | 109 | OD2 | ASP | 321 | 4.357 | 1.172 | 17.346 | 1.00 | 55.81 |
| | ATOM | 110 | C | ASP | 321 | 8.911 | 0.565 | 18.568 | 1.00 | 44.37 |
| 15 | ATOM | 111 | O | ASP | 321 | 9.030 | -0.661 | 18.533 | 1.00 | 44.67 |
| | ATOM | 112 | N | ALA | 322 | 9.878 | 1.395 | 18.193 | 1.00 | 40.75 |
| | ATOM | 113 | CA | ALA | 322 | 11.153 | 0.905 | 17.686 | 1.00 | 37.81 |
| | ATOM | 114 | CB | ALA | 322 | 11.772 | 1.954 | 16.776 | 1.00 | 38.07 |
| | ATOM | 115 | C | ALA | 322 | 12.148 | 0.513 | 18.769 | 1.00 | 35.52 |
| 20 | ATOM | 116 | O | ALA | 322 | 13.219 | -0.020 | 18.473 | 1.00 | 36.11 |
| | ATOM | 117 | N | GLU | 323 | 11.799 | 0.768 | 20.022 | 1.00 | 35.61 |
| | ATOM | 118 | CA | GLU | 323 | 12.704 | 0.460 | 21.117 | 1.00 | 36.39 |
| | ATOM | 119 | CB | GLU | 323 | 12.042 | 0.768 | 22.459 | 1.00 | 35.09 |
| | ATOM | 120 | CG | GLU | 323 | 12.209 | 2.210 | 22.899 | 1.00 | 37.93 |
| 25 | ATOM | 121 | CD | GLU | 323 | 13.657 | 2.569 | 23.200 | 1.00 | 37.29 |
| | ATOM | 122 | OE1 | GLU | 323 | 14.313 | 3.173 | 22.326 | 1.00 | 34.21 |
| | ATOM | 123 | OE2 | GLU | 323 | 14.134 | 2.245 | 24.309 | 1.00 | 38.02 |
| | ATOM | 124 | C | GLU | 323 | 13.205 | -0.978 | 21.110 | 1.00 | 38.01 |
| | ATOM | 125 | O | GLU | 323 | 12.425 | -1.931 | 20.999 | 1.00 | 38.37 |
| 30 | ATOM | 126 | N | PRO | 324 | 14.527 | -1.151 | 21.225 | 1.00 | 36.03 |
| | ATOM | 127 | CD | PRO | 324 | 15.522 | -0.069 | 21.345 | 1.00 | 36.69 |
| | ATOM | 128 | CA | PRO | 324 | 15.158 | -2.474 | 21.240 | 1.00 | 36.42 |
| | ATOM | 129 | CB | PRO | 324 | 16.633 | -2.166 | 21.003 | 1.00 | 35.75 |
| | ATOM | 130 | CG | PRO | 324 | 16.811 | -0.807 | 21.610 | 1.00 | 35.46 |
| 35 | ATOM | 131 | C | PRO | 324 | 14.940 | -3.162 | 22.583 | 1.00 | 35.75 |
| | ATOM | 132 | O | PRO | 324 | 14.616 | -2.517 | 23.580 | 1.00 | 34.97 |
| | ATOM | 133 | N | PRO | 325 | 15.134 | -4.485 | 22.631 | 1.00 | 35.24 |
| | ATOM | 134 | CD | PRO | 325 | 15.530 | -5.386 | 21.534 | 1.00 | 37.02 |
| | ATOM | 135 | CA | PRO | 325 | 14.942 | -5.208 | 23.889 | 1.00 | 34.65 |
| 40 | ATOM | 136 | CB | PRO | 325 | 14.753 | -6.652 | 23.439 | 1.00 | 35.83 |
| | ATOM | 137 | CG | PRO | 325 | 15.589 | -6.743 | 22.200 | 1.00 | 34.88 |
| | ATOM | 138 | C | PRO | 325 | 16.132 | -5.070 | 24.824 | 1.00 | 34.51 |
| | ATOM | 139 | O | PRO | 325 | 17.237 | -4.723 | 24.399 | 1.00 | 29.92 |
| | ATOM | 140 | N | ILE | 326 | 15.899 | -5.322 | 26.106 | 1.00 | 33.62 |
| 45 | ATOM | 141 | CA | ILE | 326 | 16.975 | -5.265 | 27.075 | 1.00 | 35.02 |
| | ATOM | 142 | CB | ILE | 326 | 16.458 | -4.891 | 28.473 | 1.00 | 38.11 |
| | ATOM | 143 | CG2 | ILE | 326 | 17.557 | -5.110 | 29.504 | 1.00 | 38.70 |
| | ATOM | 144 | CG1 | ILE | 326 | 15.987 | -3.431 | 28.466 | 1.00 | 40.48 |
| | ATOM | 145 | CD1 | ILE | 326 | 16.035 | -2.747 | 29.815 | 1.00 | 42.96 |
| 50 | ATOM | 146 | C | ILE | 326 | 17.567 | -6.668 | 27.103 | 1.00 | 34.14 |
| | ATOM | 147 | O | ILE | 326 | 16.875 | -7.634 | 27.427 | 1.00 | 34.88 |
| | ATOM | 148 | N | LEU | 327 | 18.840 | -6.784 | 26.745 | 1.00 | 29.64 |
| | ATOM | 149 | CA | LEU | 327 | 19.493 | -8.083 | 26.716 | 1.00 | 29.54 |
| | ATOM | 150 | CB | LEU | 327 | 20.528 | -8.135 | 25.587 | 1.00 | 27.76 |
| 55 | ATOM | 151 | CG | LEU | 327 | 19.978 | -7.800 | 24.196 | 1.00 | 29.02 |
| | ATOM | 152 | CD1 | LEU | 327 | 21.068 | -7.993 | 23.139 | 1.00 | 28.76 |
| | ATOM | 153 | CD2 | LEU | 327 | 18.775 | -8.688 | 23.891 | 1.00 | 31.26 |
| | ATOM | 154 | C | LEU | 327 | 20.156 | -8.438 | 28.030 | 1.00 | 31.21 |
| | ATOM | 155 | O | LEU | 327 | 20.393 | -7.578 | 28.891 | 1.00 | 30.12 |
| 60 | ATOM | 156 | N | TYR | 328 | 20.445 | -9.725 | 28.181 | 1.00 | 30.99 |
| | ATOM | 157 | CA | TYR | 328 | 21.087 | -10.229 | 29.381 | 1.00 | 30.95 |

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|----|------|-----|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 158 | CB | TYR | 328 | 20.409 | -11.520 | 29.842 | 1.00 | 33.38 |
| | ATOM | 159 | CG | TYR | 328 | 19.194 | -11.272 | 30.686 | 1.00 | 33.05 |
| | ATOM | 160 | CD1 | TYR | 328 | 19.253 | -11.398 | 32.071 | 1.00 | 31.92 |
| | ATOM | 161 | CE1 | TYR | 328 | 18.152 | -11.114 | 32.864 | 1.00 | 36.01 |
| | ATOM | 162 | CD2 | TYR | 328 | 17.996 | -10.862 | 30.110 | 1.00 | 36.05 |
| 10 | ATOM | 163 | CE2 | TYR | 328 | 16.880 | -10.574 | 30.899 | 1.00 | 37.27 |
| | ATOM | 164 | CZ | TYR | 328 | 16.973 | -10.702 | 32.274 | 1.00 | 37.66 |
| | ATOM | 165 | OH | TYR | 328 | 15.896 | -10.397 | 33.071 | 1.00 | 44.66 |
| | ATOM | 166 | C | TYR | 328 | 22.529 | -10.520 | 29.067 | 1.00 | 33.66 |
| | ATOM | 167 | O | TYR | 328 | 22.884 | -10.744 | 27.910 | 1.00 | 34.78 |
| 15 | ATOM | 168 | N | SER | 329 | 23.359 | -10.496 | 30.103 | 1.00 | 33.97 |
| | ATOM | 169 | CA | SER | 329 | 24.767 | -10.800 | 29.962 | 1.00 | 37.29 |
| | ATOM | 170 | CB | SER | 329 | 25.526 | -10.342 | 31.204 | 1.00 | 36.51 |
| | ATOM | 171 | OG | SER | 329 | 26.787 | -10.965 | 31.282 | 1.00 | 37.13 |
| | ATOM | 172 | C | SER | 329 | 24.835 | -12.317 | 29.832 | 1.00 | 40.43 |
| 20 | ATOM | 173 | O | SER | 329 | 23.980 | -13.028 | 30.363 | 1.00 | 40.11 |
| | ATOM | 174 | N | GLU | 330 | 25.845 | -12.811 | 29.128 | 1.00 | 41.40 |
| | ATOM | 175 | CA | GLU | 330 | 25.992 | -14.242 | 28.928 | 1.00 | 47.43 |
| | ATOM | 176 | CB | GLU | 330 | 26.423 | -14.524 | 27.484 | 1.00 | 48.64 |
| | ATOM | 177 | CG | GLU | 330 | 25.278 | -14.870 | 26.542 | 1.00 | 50.20 |
| 25 | ATOM | 178 | CD | GLU | 330 | 25.765 | -15.405 | 25.198 | 1.00 | 53.25 |
| | ATOM | 179 | OE1 | GLU | 330 | 25.909 | -16.640 | 25.062 | 1.00 | 53.27 |
| | ATOM | 180 | OE2 | GLU | 330 | 26.004 | -14.590 | 24.280 | 1.00 | 51.80 |
| | ATOM | 181 | C | GLU | 330 | 26.999 | -14.852 | 29.893 | 1.00 | 49.67 |
| | ATOM | 182 | O | GLU | 330 | 28.207 | -14.741 | 29.696 | 1.00 | 50.11 |
| 30 | ATOM | 183 | N | TYR | 331 | 26.498 | -15.493 | 30.942 | 1.00 | 53.62 |
| | ATOM | 184 | CA | TYR | 331 | 27.373 | -16.130 | 31.921 | 1.00 | 58.16 |
| | ATOM | 185 | CB | TYR | 331 | 28.092 | -15.078 | 32.774 | 1.00 | 59.55 |
| | ATOM | 186 | CG | TYR | 331 | 27.239 | -14.460 | 33.860 | 1.00 | 63.08 |
| | ATOM | 187 | CD1 | TYR | 331 | 26.656 | -13.205 | 33.682 | 1.00 | 64.50 |
| 35 | ATOM | 188 | CE1 | TYR | 331 | 25.864 | -12.630 | 34.676 | 1.00 | 65.99 |
| | ATOM | 189 | CD2 | TYR | 331 | 27.010 | -15.128 | 35.065 | 1.00 | 63.52 |
| | ATOM | 190 | CE2 | TYR | 331 | 26.219 | -14.563 | 36.066 | 1.00 | 65.60 |
| | ATOM | 191 | CZ | TYR | 331 | 25.648 | -13.314 | 35.864 | 1.00 | 67.20 |
| | ATOM | 192 | OH | TYR | 331 | 24.855 | -12.753 | 36.839 | 1.00 | 67.40 |
| 40 | ATOM | 193 | C | TYR | 331 | 26.603 | -17.080 | 32.823 | 1.00 | 59.05 |
| | ATOM | 194 | O | TYR | 331 | 25.393 | -16.942 | 33.002 | 1.00 | 59.22 |
| | ATOM | 195 | N | ASP | 332 | 27.320 | -18.045 | 33.387 | 1.00 | 61.62 |
| | ATOM | 196 | CA | ASP | 332 | 26.719 | -19.026 | 34.281 | 1.00 | 64.20 |
| | ATOM | 197 | CB | ASP | 332 | 27.681 | -20.194 | 34.500 | 1.00 | 65.99 |
| 45 | ATOM | 198 | CG | ASP | 332 | 26.961 | -21.516 | 34.648 | 1.00 | 68.11 |
| | ATOM | 199 | OD1 | ASP | 332 | 27.575 | -22.564 | 34.351 | 1.00 | 69.54 |
| | ATOM | 200 | OD2 | ASP | 332 | 25.781 | -21.505 | 35.060 | 1.00 | 67.40 |
| | ATOM | 201 | C | ASP | 332 | 26.393 | -18.371 | 35.619 | 1.00 | 63.33 |
| | ATOM | 202 | O | ASP | 332 | 27.292 | -18.073 | 36.406 | 1.00 | 63.90 |
| 50 | ATOM | 203 | N | PRO | 333 | 25.096 | -18.148 | 35.896 | 1.00 | 63.64 |
| | ATOM | 204 | CD | PRO | 333 | 23.945 | -18.509 | 35.053 | 1.00 | 64.35 |
| | ATOM | 205 | CA | PRO | 333 | 24.677 | -17.521 | 37.154 | 1.00 | 63.52 |
| | ATOM | 206 | CB | PRO | 333 | 23.165 | -17.333 | 36.993 | 1.00 | 63.53 |
| | ATOM | 207 | CG | PRO | 333 | 22.866 | -17.611 | 35.556 | 1.00 | 64.15 |
| 55 | ATOM | 208 | C | PRO | 333 | 25.010 | -18.419 | 38.332 | 1.00 | 63.29 |
| | ATOM | 209 | O | PRO | 333 | 25.129 | -17.964 | 39.468 | 1.00 | 63.28 |
| | ATOM | 210 | N | THR | 334 | 25.160 | -19.704 | 38.037 | 1.00 | 64.26 |
| | ATOM | 211 | CA | THR | 334 | 25.475 | -20.697 | 39.050 | 1.00 | 66.09 |
| | ATOM | 212 | CB | THR | 334 | 24.929 | -22.080 | 38.645 | 1.00 | 66.90 |
| 60 | ATOM | 213 | OG1 | THR | 334 | 25.571 | -22.513 | 37.439 | 1.00 | 68.06 |
| | ATOM | 214 | CG2 | THR | 334 | 23.423 | -22.012 | 38.411 | 1.00 | 67.57 |

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|----|------|-----|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 215 | C | THR | 334 | 26.982 | -20.804 | 39.269 | 1.00 | 65.67 |
| | ATOM | 216 | O | THR | 334 | 27.432 | -21.323 | 40.289 | 1.00 | 64.77 |
| | ATOM | 217 | N | ARG | 335 | 27.759 | -20.308 | 38.313 | 1.00 | 65.65 |
| | ATOM | 218 | CA | ARG | 335 | 29.214 | -20.360 | 38.421 | 1.00 | 66.60 |
| | ATOM | 219 | CB | ARG | 335 | 29.835 | -20.500 | 37.030 | 1.00 | 66.74 |
| 10 | ATOM | 220 | C | ARG | 335 | 29.757 | -19.113 | 39.123 | 1.00 | 67.09 |
| | ATOM | 221 | O | ARG | 335 | 29.100 | -18.071 | 39.148 | 1.00 | 67.31 |
| | ATOM | 222 | N | PRO | 336 | 30.968 | -19.207 | 39.702 | 1.00 | 67.62 |
| | ATOM | 223 | CD | PRO | 336 | 31.820 | -20.408 | 39.713 | 1.00 | 67.30 |
| | ATOM | 224 | CA | PRO | 336 | 31.601 | -18.086 | 40.410 | 1.00 | 67.42 |
| 15 | ATOM | 225 | CB | PRO | 336 | 32.982 | -18.621 | 40.783 | 1.00 | 66.43 |
| | ATOM | 226 | CG | PRO | 336 | 32.829 | -20.097 | 40.779 | 1.00 | 67.52 |
| | ATOM | 227 | C | PRO | 336 | 31.701 | -16.828 | 39.561 | 1.00 | 68.26 |
| | ATOM | 228 | O | PRO | 336 | 31.996 | -16.895 | 38.371 | 1.00 | 69.04 |
| | ATOM | 229 | N | PHE | 337 | 31.460 | -15.681 | 40.183 | 1.00 | 69.49 |
| 20 | ATOM | 230 | CA | PHE | 337 | 31.529 | -14.408 | 39.480 | 1.00 | 71.39 |
| | ATOM | 231 | CB | PHE | 337 | 30.818 | -13.323 | 40.294 | 1.00 | 72.31 |
| | ATOM | 232 | CG | PHE | 337 | 31.219 | -11.924 | 39.921 | 1.00 | 73.21 |
| | ATOM | 233 | CD1 | PHE | 337 | 30.632 | -11.287 | 38.833 | 1.00 | 72.82 |
| | ATOM | 234 | CD2 | PHE | 337 | 32.191 | -11.245 | 40.653 | 1.00 | 73.43 |
| 25 | ATOM | 235 | CE1 | PHE | 337 | 31.006 | -9.993 | 38.479 | 1.00 | 73.28 |
| | ATOM | 236 | CE2 | PHE | 337 | 32.573 | -9.950 | 40.306 | 1.00 | 73.00 |
| | ATOM | 237 | CZ | PHE | 337 | 31.980 | -9.323 | 39.217 | 1.00 | 72.90 |
| | ATOM | 238 | C | PHE | 337 | 32.985 | -14.013 | 39.245 | 1.00 | 71.38 |
| | ATOM | 239 | O | PHE | 337 | 33.336 | -13.487 | 38.189 | 1.00 | 71.56 |
| 30 | ATOM | 240 | N | SER | 338 | 33.825 | -14.273 | 40.241 | 1.00 | 71.53 |
| | ATOM | 241 | CA | SER | 338 | 35.248 | -13.947 | 40.172 | 1.00 | 70.98 |
| | ATOM | 242 | CB | SER | 338 | 35.957 | -14.487 | 41.414 | 1.00 | 70.43 |
| | ATOM | 243 | OG | SER | 338 | 35.547 | -15.818 | 41.679 | 1.00 | 69.59 |
| | ATOM | 244 | C | SER | 338 | 35.931 | -14.504 | 38.924 | 1.00 | 71.20 |
| 35 | ATOM | 245 | O | SER | 338 | 36.951 | -13.972 | 38.475 | 1.00 | 71.35 |
| | ATOM | 246 | N | GLU | 339 | 35.368 | -15.573 | 38.369 | 1.00 | 70.20 |
| | ATOM | 247 | CA | GLU | 339 | 35.930 | -16.215 | 37.183 | 1.00 | 69.48 |
| | ATOM | 248 | CB | GLU | 339 | 35.279 | -17.585 | 36.971 | 1.00 | 71.07 |
| | ATOM | 249 | CG | GLU | 339 | 35.996 | -18.740 | 37.656 | 1.00 | 72.60 |
| 40 | ATOM | 250 | CD | GLU | 339 | 35.382 | -20.089 | 37.318 | 1.00 | 74.26 |
| | ATOM | 251 | OE1 | GLU | 339 | 34.786 | -20.220 | 36.227 | 1.00 | 73.51 |
| | ATOM | 252 | OE2 | GLU | 339 | 35.496 | -21.020 | 38.144 | 1.00 | 76.44 |
| | ATOM | 253 | C | GLU | 339 | 35.770 | -15.385 | 35.910 | 1.00 | 68.15 |
| | ATOM | 254 | O | GLU | 339 | 36.722 | -15.216 | 35.144 | 1.00 | 68.99 |
| 45 | ATOM | 255 | N | ALA | 340 | 34.562 | -14.874 | 35.694 | 1.00 | 64.41 |
| | ATOM | 256 | CA | ALA | 340 | 34.246 | -14.083 | 34.507 | 1.00 | 60.69 |
| | ATOM | 257 | CB | ALA | 340 | 32.767 | -13.709 | 34.523 | 1.00 | 61.17 |
| | ATOM | 258 | C | ALA | 340 | 35.096 | -12.824 | 34.326 | 1.00 | 57.00 |
| | ATOM | 259 | O | ALA | 340 | 35.634 | -12.270 | 35.287 | 1.00 | 57.46 |
| 50 | ATOM | 260 | N | SER | 341 | 35.215 | -12.388 | 33.076 | 1.00 | 52.15 |
| | ATOM | 261 | CA | SER | 341 | 35.972 | -11.188 | 32.736 | 1.00 | 46.53 |
| | ATOM | 262 | CB | SER | 341 | 36.839 | -11.439 | 31.497 | 1.00 | 48.64 |
| | ATOM | 263 | OG | SER | 341 | 37.184 | -10.226 | 30.846 | 1.00 | 46.48 |
| | ATOM | 264 | C | SER | 341 | 34.957 | -10.087 | 32.444 | 1.00 | 43.52 |
| 55 | ATOM | 265 | O | SER | 341 | 34.090 | -10.248 | 31.589 | 1.00 | 39.92 |
| | ATOM | 266 | N | MET | 342 | 35.052 | -8.978 | 33.166 | 1.00 | 41.24 |
| | ATOM | 267 | CA | MET | 342 | 34.121 | -7.875 | 32.960 | 1.00 | 42.46 |
| | ATOM | 268 | CB | MET | 342 | 34.449 | -6.723 | 33.912 | 1.00 | 45.61 |
| | ATOM | 269 | CG | MET | 342 | 33.228 | -6.089 | 34.560 | 1.00 | 52.39 |
| 60 | ATOM | 270 | SD | MET | 342 | 31.791 | -7.201 | 34.631 | 1.00 | 57.92 |
| | ATOM | 271 | CE | MET | 342 | 31.999 | -7.881 | 36.239 | 1.00 | 56.18 |

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|----|------|-----|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 272 | C | MET | 342 | 34.124 | -7.365 | 31.516 | 1.00 | 40.22 |
| | ATOM | 273 | O | MET | 342 | 33.063 | -7.121 | 30.938 | 1.00 | 39.23 |
| | ATOM | 274 | N | MET | 343 | 35.307 | -7.204 | 30.930 | 1.00 | 38.72 |
| | ATOM | 275 | CA | MET | 343 | 35.395 | -6.708 | 29.558 | 1.00 | 38.50 |
| | ATOM | 276 | CB | MET | 343 | 36.838 | -6.318 | 29.216 | 1.00 | 41.15 |
| 10 | ATOM | 277 | CG | MET | 343 | 37.022 | -5.749 | 27.804 | 1.00 | 40.31 |
| | ATOM | 278 | SD | MET | 343 | 36.032 | -4.260 | 27.427 | 1.00 | 45.23 |
| | ATOM | 279 | CE | MET | 343 | 36.113 | -3.358 | 28.987 | 1.00 | 40.45 |
| | ATOM | 280 | C | MET | 343 | 34.880 | -7.741 | 28.561 | 1.00 | 35.36 |
| | ATOM | 281 | O | MET | 343 | 34.368 | -7.384 | 27.501 | 1.00 | 35.51 |
| 15 | ATOM | 282 | N | GLY | 344 | 35.017 | -9.020 | 28.902 | 1.00 | 35.53 |
| | ATOM | 283 | CA | GLY | 344 | 34.533 | -10.072 | 28.024 | 1.00 | 33.41 |
| | ATOM | 284 | C | GLY | 344 | 33.015 | -10.063 | 28.047 | 1.00 | 31.74 |
| | ATOM | 285 | O | GLY | 344 | 32.359 | -10.233 | 27.019 | 1.00 | 29.58 |
| | ATOM | 286 | N | LEU | 345 | 32.459 | -9.860 | 29.238 | 1.00 | 32.89 |
| 20 | ATOM | 287 | CA | LEU | 345 | 31.011 | -9.804 | 29.415 | 1.00 | 34.95 |
| | ATOM | 288 | CB | LEU | 345 | 30.665 | -9.631 | 30.902 | 1.00 | 37.56 |
| | ATOM | 289 | CG | LEU | 345 | 30.942 | -10.774 | 31.883 | 1.00 | 43.03 |
| | ATOM | 290 | CD1 | LEU | 345 | 30.537 | -10.357 | 33.297 | 1.00 | 41.57 |
| | ATOM | 291 | CD2 | LEU | 345 | 30.164 | -11.998 | 31.449 | 1.00 | 42.80 |
| 25 | ATOM | 292 | C | LEU | 345 | 30.430 | -8.614 | 28.633 | 1.00 | 33.71 |
| | ATOM | 293 | O | LEU | 345 | 29.479 | -8.757 | 27.868 | 1.00 | 30.29 |
| | ATOM | 294 | N | LEU | 346 | 31.021 | -7.443 | 28.843 | 1.00 | 30.20 |
| | ATOM | 295 | CA | LEU | 346 | 30.569 | -6.217 | 28.193 | 1.00 | 32.00 |
| | ATOM | 296 | CB | LEU | 346 | 31.317 | -5.016 | 28.771 | 1.00 | 28.16 |
| 30 | ATOM | 297 | CG | LEU | 346 | 31.091 | -4.767 | 30.269 | 1.00 | 29.84 |
| | ATOM | 298 | CD1 | LEU | 346 | 31.815 | -3.498 | 30.668 | 1.00 | 29.98 |
| | ATOM | 299 | CD2 | LEU | 346 | 29.614 | -4.644 | 30.581 | 1.00 | 33.97 |
| | ATOM | 300 | C | LEU | 346 | 30.732 | -6.250 | 26.682 | 1.00 | 30.70 |
| | ATOM | 301 | O | LEU | 346 | 29.869 | -5.765 | 25.955 | 1.00 | 29.13 |
| 35 | ATOM | 302 | N | THR | 347 | 31.839 | -6.816 | 26.212 | 1.00 | 30.47 |
| | ATOM | 303 | CA | THR | 347 | 32.086 | -6.911 | 24.781 | 1.00 | 30.93 |
| | ATOM | 304 | CB | THR | 347 | 33.472 | -7.501 | 24.497 | 1.00 | 29.97 |
| | ATOM | 305 | OG1 | THR | 347 | 34.481 | -6.604 | 24.982 | 1.00 | 35.40 |
| | ATOM | 306 | CG2 | THR | 347 | 33.666 | -7.707 | 23.004 | 1.00 | 33.58 |
| 40 | ATOM | 307 | C | THR | 347 | 31.036 | -7.804 | 24.122 | 1.00 | 31.97 |
| | ATOM | 308 | O | THR | 347 | 30.516 | -7.486 | 23.049 | 1.00 | 30.75 |
| | ATOM | 309 | N | ASN | 348 | 30.737 | -8.926 | 24.768 | 1.00 | 29.31 |
| | ATOM | 310 | CA | ASN | 348 | 29.757 | -9.868 | 24.242 | 1.00 | 32.63 |
| | ATOM | 311 | CB | ASN | 348 | 29.767 | -11.161 | 25.065 | 1.00 | 31.64 |
| 45 | ATOM | 312 | CG | ASN | 348 | 28.646 | -12.117 | 24.662 | 1.00 | 39.14 |
| | ATOM | 313 | OD1 | ASN | 348 | 27.549 | -12.078 | 25.220 | 1.00 | 41.91 |
| | ATOM | 314 | ND2 | ASN | 348 | 28.920 | -12.970 | 23.683 | 1.00 | 42.05 |
| | ATOM | 315 | C | ASN | 348 | 28.361 | -9.251 | 24.262 | 1.00 | 29.02 |
| | ATOM | 316 | O | ASN | 348 | 27.558 | -9.477 | 23.353 | 1.00 | 32.76 |
| 50 | ATOM | 317 | N | LEU | 349 | 28.078 | -8.467 | 25.298 | 1.00 | 28.74 |
| | ATOM | 318 | CA | LEU | 349 | 26.782 | -7.811 | 25.421 | 1.00 | 28.58 |
| | ATOM | 319 | CB | LEU | 349 | 26.650 | -7.148 | 26.795 | 1.00 | 26.56 |
| | ATOM | 320 | CG | LEU | 349 | 25.376 | -6.328 | 27.050 | 1.00 | 33.67 |
| | ATOM | 321 | CD1 | LEU | 349 | 24.140 | -7.199 | 26.840 | 1.00 | 28.82 |
| 55 | ATOM | 322 | CD2 | LEU | 349 | 25.392 | -5.779 | 28.471 | 1.00 | 33.11 |
| | ATOM | 323 | C | LEU | 349 | 26.638 | -6.762 | 24.319 | 1.00 | 28.07 |
| | ATOM | 324 | O | LEU | 349 | 25.616 | -6.703 | 23.629 | 1.00 | 25.22 |
| | ATOM | 325 | N | ALA | 350 | 27.675 | -5.941 | 24.157 | 1.00 | 28.50 |
| | ATOM | 326 | CA | ALA | 350 | 27.668 | -4.886 | 23.148 | 1.00 | 28.46 |
| 60 | ATOM | 327 | CB | ALA | 350 | 28.972 | -4.094 | 23.209 | 1.00 | 28.12 |
| | ATOM | 328 | C | ALA | 350 | 27.468 | -5.461 | 21.750 | 1.00 | 28.75 |

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|----|------|-----|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 329 | O | ALA | 350 | 26.649 | -4.958 | 20.983 | 1.00 | 30.90 |
| | ATOM | 330 | N | ASP | 351 | 28.213 | -6.509 | 21.420 | 1.00 | 27.20 |
| | ATOM | 331 | CA | ASP | 351 | 28.093 | -7.143 | 20.112 | 1.00 | 29.75 |
| | ATOM | 332 | CB | ASP | 351 | 29.036 | -8.345 | 20.010 | 1.00 | 34.16 |
| | ATOM | 333 | CG | ASP | 351 | 30.498 | -7.940 | 19.978 | 1.00 | 37.50 |
| 10 | ATOM | 334 | OD1 | ASP | 351 | 31.354 | -8.831 | 20.148 | 1.00 | 37.55 |
| | ATOM | 335 | OD2 | ASP | 351 | 30.789 | -6.738 | 19.784 | 1.00 | 35.50 |
| | ATOM | 336 | C | ASP | 351 | 26.661 | -7.600 | 19.813 | 1.00 | 30.52 |
| | ATOM | 337 | O | ASP | 351 | 26.193 | -7.458 | 18.687 | 1.00 | 27.77 |
| | ATOM | 338 | N | ARG | 352 | 25.968 | -8.150 | 20.811 | 1.00 | 27.18 |
| 15 | ATOM | 339 | CA | ARG | 352 | 24.593 | -8.602 | 20.605 | 1.00 | 26.21 |
| | ATOM | 340 | CB | ARG | 352 | 24.148 | -9.534 | 21.752 | 1.00 | 26.52 |
| | ATOM | 341 | CG | ARG | 352 | 24.567 | -10.991 | 21.532 | 1.00 | 31.03 |
| | ATOM | 342 | CD | ARG | 352 | 24.128 | -11.911 | 22.666 | 1.00 | 29.80 |
| | ATOM | 343 | NE | ARG | 352 | 24.898 | -11.675 | 23.879 | 1.00 | 30.44 |
| 20 | ATOM | 344 | CZ | ARG | 352 | 24.364 | -11.363 | 25.054 | 1.00 | 31.68 |
| | ATOM | 345 | NH1 | ARG | 352 | 23.050 | -11.251 | 25.177 | 1.00 | 31.18 |
| | ATOM | 346 | NH2 | ARG | 352 | 25.144 | -11.148 | 26.104 | 1.00 | 32.03 |
| | ATOM | 347 | C | ARG | 352 | 23.642 | -7.411 | 20.502 | 1.00 | 27.16 |
| | ATOM | 348 | O | ARG | 352 | 22.702 | -7.426 | 19.708 | 1.00 | 26.65 |
| 25 | ATOM | 349 | N | GLU | 353 | 23.896 | -6.370 | 21.291 | 1.00 | 24.30 |
| | ATOM | 350 | CA | GLU | 353 | 23.045 | -5.178 | 21.261 | 1.00 | 26.39 |
| | ATOM | 351 | CB | GLU | 353 | 23.461 | -4.204 | 22.365 | 1.00 | 24.91 |
| | ATOM | 352 | CG | GLU | 353 | 23.147 | -4.669 | 23.771 | 1.00 | 27.93 |
| | ATOM | 353 | CD | GLU | 353 | 23.425 | -3.587 | 24.795 | 1.00 | 30.71 |
| 30 | ATOM | 354 | OE1 | GLU | 353 | 24.564 | -3.534 | 25.304 | 1.00 | 30.09 |
| | ATOM | 355 | OE2 | GLU | 353 | 22.506 | -2.789 | 25.085 | 1.00 | 30.53 |
| | ATOM | 356 | C | GLU | 353 | 23.131 | -4.456 | 19.920 | 1.00 | 24.27 |
| | ATOM | 357 | O | GLU | 353 | 22.169 | -3.826 | 19.467 | 1.00 | 28.71 |
| | ATOM | 358 | N | LEU | 354 | 24.296 | -4.540 | 19.293 | 1.00 | 26.61 |
| 35 | ATOM | 359 | CA | LEU | 354 | 24.522 | -3.872 | 18.017 | 1.00 | 26.62 |
| | ATOM | 360 | CB | LEU | 354 | 25.952 | -4.121 | 17.543 | 1.00 | 26.36 |
| | ATOM | 361 | CG | LEU | 354 | 26.372 | -3.257 | 16.351 | 1.00 | 29.24 |
| | ATOM | 362 | CD1 | LEU | 354 | 26.243 | -1.774 | 16.722 | 1.00 | 26.59 |
| | ATOM | 363 | CD2 | LEU | 354 | 27.794 | -3.607 | 15.962 | 1.00 | 28.88 |
| 40 | ATOM | 364 | C | LEU | 354 | 23.559 | -4.300 | 16.926 | 1.00 | 27.72 |
| | ATOM | 365 | O | LEU | 354 | 23.074 | -3.475 | 16.152 | 1.00 | 24.00 |
| | ATOM | 366 | N | VAL | 355 | 23.291 | -5.598 | 16.854 | 1.00 | 28.82 |
| | ATOM | 367 | CA | VAL | 355 | 22.386 | -6.125 | 15.844 | 1.00 | 29.45 |
| | ATOM | 368 | CB | VAL | 355 | 22.259 | -7.655 | 15.975 | 1.00 | 31.76 |
| 45 | ATOM | 369 | CG1 | VAL | 355 | 21.423 | -8.205 | 14.834 | 1.00 | 33.55 |
| | ATOM | 370 | CG2 | VAL | 355 | 23.649 | -8.282 | 15.998 | 1.00 | 31.36 |
| | ATOM | 371 | C | VAL | 355 | 21.020 | -5.499 | 16.035 | 1.00 | 27.71 |
| | ATOM | 372 | O | VAL | 355 | 20.382 | -5.039 | 15.080 | 1.00 | 29.61 |
| | ATOM | 373 | N | HIS | 356 | 20.580 | -5.473 | 17.288 | 1.00 | 27.76 |
| 50 | ATOM | 374 | CA | HIS | 356 | 19.291 | -4.906 | 17.627 | 1.00 | 28.35 |
| | ATOM | 375 | CB | HIS | 356 | 18.936 | -5.231 | 19.079 | 1.00 | 31.12 |
| | ATOM | 376 | CG | HIS | 356 | 18.602 | -6.675 | 19.307 | 1.00 | 35.93 |
| | ATOM | 377 | CD2 | HIS | 356 | 19.352 | -7.700 | 19.779 | 1.00 | 33.95 |
| | ATOM | 378 | ND1 | HIS | 356 | 17.363 | -7.208 | 19.018 | 1.00 | 36.62 |
| 55 | ATOM | 379 | CE1 | HIS | 356 | 17.364 | -8.499 | 19.304 | 1.00 | 33.33 |
| | ATOM | 380 | NE2 | HIS | 356 | 18.559 | -8.823 | 19.767 | 1.00 | 32.16 |
| | ATOM | 381 | C | HIS | 356 | 19.300 | -3.398 | 17.412 | 1.00 | 28.25 |
| | ATOM | 382 | O | HIS | 356 | 18.272 | -2.812 | 17.100 | 1.00 | 28.99 |
| | ATOM | 383 | N | MET | 357 | 20.457 | -2.765 | 17.574 | 1.00 | 25.31 |
| 60 | ATOM | 384 | CA | MET | 357 | 20.526 | -1.322 | 17.369 | 1.00 | 24.63 |
| | ATOM | 385 | CB | MET | 357 | 21.902 | -0.789 | 17.766 | 1.00 | 23.61 |

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|----|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 386 | CG | MET | 357 | 22.011 | 0.736 | 17.699 | 1.00 | 24.66 |
| | ATOM | 387 | SD | MET | 357 | 23.732 | 1.290 | 17.859 | 1.00 | 27.30 |
| | ATOM | 388 | CE | MET | 357 | 24.140 | 0.672 | 19.514 | 1.00 | 23.62 |
| | ATOM | 389 | C | MET | 357 | 20.256 | -1.011 | 15.898 | 1.00 | 24.83 |
| | ATOM | 390 | O | MET | 357 | 19.619 | -0.003 | 15.569 | 1.00 | 26.78 |
| 10 | ATOM | 391 | N | ILE | 358 | 20.757 | -1.874 | 15.020 | 1.00 | 26.25 |
| | ATOM | 392 | CA | ILE | 358 | 20.553 | -1.721 | 13.576 | 1.00 | 30.33 |
| | ATOM | 393 | CB | ILE | 358 | 21.204 | -2.888 | 12.789 | 1.00 | 33.86 |
| | ATOM | 394 | CG2 | ILE | 358 | 20.759 | -2.860 | 11.334 | 1.00 | 33.68 |
| | ATOM | 395 | CG1 | ILE | 358 | 22.728 | -2.799 | 12.874 | 1.00 | 36.89 |
| 15 | ATOM | 396 | CD1 | ILE | 358 | 23.299 | -1.469 | 12.451 | 1.00 | 39.10 |
| | ATOM | 397 | C | ILE | 358 | 19.055 | -1.721 | 13.310 | 1.00 | 32.20 |
| | ATOM | 398 | O | ILE | 358 | 18.519 | -0.817 | 12.662 | 1.00 | 32.02 |
| | ATOM | 399 | N | ASN | 359 | 18.379 | -2.748 | 13.814 | 1.00 | 33.12 |
| | ATOM | 400 | CA | ASN | 359 | 16.945 | -2.861 | 13.638 | 1.00 | 33.35 |
| 20 | ATOM | 401 | CB | ASN | 359 | 16.434 | -4.101 | 14.363 | 1.00 | 37.59 |
| | ATOM | 402 | CG | ASN | 359 | 16.739 | -5.374 | 13.627 | 1.00 | 44.38 |
| | ATOM | 403 | OD1 | ASN | 359 | 17.045 | -5.329 | 12.437 | 1.00 | 47.35 |
| | ATOM | 404 | ND2 | ASN | 359 | 16.673 | -6.508 | 14.320 | 1.00 | 42.48 |
| | ATOM | 405 | C | ASN | 359 | 16.224 | -1.634 | 14.149 | 1.00 | 32.74 |
| 25 | ATOM | 406 | O | ASN | 359 | 15.261 | -1.163 | 13.530 | 1.00 | 31.39 |
| | ATOM | 407 | N | TRP | 360 | 16.706 | -1.104 | 15.264 | 1.00 | 27.92 |
| | ATOM | 408 | CA | TRP | 360 | 16.102 | 0.087 | 15.842 | 1.00 | 29.47 |
| | ATOM | 409 | CB | TRP | 360 | 16.703 | 0.347 | 17.228 | 1.00 | 27.66 |
| | ATOM | 410 | CG | TRP | 360 | 16.522 | 1.747 | 17.707 | 1.00 | 30.40 |
| 30 | ATOM | 411 | CD2 | TRP | 360 | 17.493 | 2.801 | 17.657 | 1.00 | 27.54 |
| | ATOM | 412 | CE2 | TRP | 360 | 16.888 | 3.954 | 18.204 | 1.00 | 29.42 |
| | ATOM | 413 | CE3 | TRP | 360 | 18.819 | 2.883 | 17.205 | 1.00 | 28.37 |
| | ATOM | 414 | CD1 | TRP | 360 | 15.399 | 2.284 | 18.264 | 1.00 | 27.75 |
| | ATOM | 415 | NE1 | TRP | 360 | 15.609 | 3.611 | 18.566 | 1.00 | 30.84 |
| 35 | ATOM | 416 | CZ2 | TRP | 360 | 17.558 | 5.180 | 18.310 | 1.00 | 27.74 |
| | ATOM | 417 | CZ3 | TRP | 360 | 19.488 | 4.106 | 17.309 | 1.00 | 24.49 |
| | ATOM | 418 | CH2 | TRP | 360 | 18.853 | 5.232 | 17.858 | 1.00 | 25.09 |
| | ATOM | 419 | C | TRP | 360 | 16.312 | 1.296 | 14.926 | 1.00 | 27.90 |
| | ATOM | 420 | O | TRP | 360 | 15.360 | 2.002 | 14.581 | 1.00 | 28.83 |
| 40 | ATOM | 421 | N | ALA | 361 | 17.559 | 1.520 | 14.523 | 1.00 | 28.25 |
| | ATOM | 422 | CA | ALA | 361 | 17.894 | 2.637 | 13.645 | 1.00 | 29.20 |
| | ATOM | 423 | CB | ALA | 361 | 19.346 | 2.539 | 13.220 | 1.00 | 28.89 |
| | ATOM | 424 | C | ALA | 361 | 17.006 | 2.685 | 12.403 | 1.00 | 31.08 |
| | ATOM | 425 | O | ALA | 361 | 16.531 | 3.746 | 12.011 | 1.00 | 31.30 |
| 45 | ATOM | 426 | N | LYS | 362 | 16.795 | 1.526 | 11.783 | 1.00 | 30.93 |
| | ATOM | 427 | CA | LYS | 362 | 15.981 | 1.443 | 10.581 | 1.00 | 34.15 |
| | ATOM | 428 | CB | LYS | 362 | 16.012 | 0.016 | 10.023 | 1.00 | 33.67 |
| | ATOM | 429 | CG | LYS | 362 | 17.252 | -0.281 | 9.198 | 1.00 | 39.40 |
| | ATOM | 430 | CD | LYS | 362 | 17.547 | -1.774 | 9.136 | 1.00 | 43.60 |
| 50 | ATOM | 431 | CE | LYS | 362 | 18.852 | -2.046 | 8.389 | 1.00 | 47.06 |
| | ATOM | 432 | NZ | LYS | 362 | 19.178 | -3.507 | 8.288 | 1.00 | 50.34 |
| | ATOM | 433 | C | LYS | 362 | 14.545 | 1.872 | 10.815 | 1.00 | 35.81 |
| | ATOM | 434 | O | LYS | 362 | 13.821 | 2.168 | 9.859 | 1.00 | 37.95 |
| | ATOM | 435 | N | ARG | 363 | 14.134 | 1.921 | 12.079 | 1.00 | 34.23 |
| 55 | ATOM | 436 | CA | ARG | 363 | 12.770 | 2.313 | 12.409 | 1.00 | 36.04 |
| | ATOM | 437 | CB | ARG | 363 | 12.178 | 1.307 | 13.391 | 1.00 | 36.71 |
| | ATOM | 438 | CG | ARG | 363 | 12.169 | -0.110 | 12.827 | 1.00 | 40.36 |
| | ATOM | 439 | CD | ARG | 363 | 11.468 | -1.086 | 13.746 | 1.00 | 42.17 |
| | ATOM | 440 | NE | ARG | 363 | 10.161 | -0.586 | 14.158 | 1.00 | 45.19 |
| 60 | ATOM | 441 | CZ | ARG | 363 | 9.314 | -1.262 | 14.929 | 1.00 | 49.41 |
| | ATOM | 442 | NH1 | ARG | 363 | 9.642 | -2.467 | 15.374 | 1.00 | 48.02 |

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|----|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 443 | NH2 | ARG | 363 | 8.143 | -0.729 | 15.261 | 1.00 | 51.54 |
| | ATOM | 444 | C | ARG | 363 | 12.654 | 3.743 | 12.943 | 1.00 | 37.40 |
| | ATOM | 445 | O | ARG | 363 | 11.567 | 4.199 | 13.303 | 1.00 | 38.22 |
| | ATOM | 446 | N | VAL | 364 | 13.785 | 4.442 | 13.002 | 1.00 | 35.66 |
| | ATOM | 447 | CA | VAL | 364 | 13.804 | 5.836 | 13.431 | 1.00 | 34.06 |
| 10 | ATOM | 448 | CB | VAL | 364 | 15.231 | 6.271 | 13.827 | 1.00 | 33.87 |
| | ATOM | 449 | CG1 | VAL | 364 | 15.293 | 7.779 | 13.995 | 1.00 | 31.08 |
| | ATOM | 450 | CG2 | VAL | 364 | 15.641 | 5.571 | 15.113 | 1.00 | 31.30 |
| | ATOM | 451 | C | VAL | 364 | 13.360 | 6.591 | 12.171 | 1.00 | 33.19 |
| | ATOM | 452 | O | VAL | 364 | 14.028 | 6.531 | 11.146 | 1.00 | 33.04 |
| 15 | ATOM | 453 | N | PRO | 365 | 12.225 | 7.310 | 12.234 | 1.00 | 34.69 |
| | ATOM | 454 | CD | PRO | 365 | 11.359 | 7.492 | 13.413 | 1.00 | 34.19 |
| | ATOM | 455 | CA | PRO | 365 | 11.724 | 8.050 | 11.069 | 1.00 | 35.96 |
| | ATOM | 456 | CB | PRO | 365 | 10.608 | 8.918 | 11.645 | 1.00 | 36.59 |
| | ATOM | 457 | CG | PRO | 365 | 10.135 | 8.157 | 12.842 | 1.00 | 39.59 |
| 20 | ATOM | 458 | C | PRO | 365 | 12.756 | 8.878 | 10.321 | 1.00 | 37.19 |
| | ATOM | 459 | O | PRO | 365 | 13.430 | 9.726 | 10.907 | 1.00 | 40.29 |
| | ATOM | 460 | N | GLY | 366 | 12.878 | 8.624 | 9.023 | 1.00 | 34.78 |
| | ATOM | 461 | CA | GLY | 366 | 13.816 | 9.371 | 8.212 | 1.00 | 33.54 |
| | ATOM | 462 | C | GLY | 366 | 15.168 | 8.722 | 8.007 | 1.00 | 34.26 |
| 25 | ATOM | 463 | O | GLY | 366 | 15.858 | 9.035 | 7.034 | 1.00 | 37.15 |
| | ATOM | 464 | N | PHE | 367 | 15.554 | 7.814 | 8.901 | 1.00 | 33.13 |
| | ATOM | 465 | CA | PHE | 367 | 16.860 | 7.164 | 8.787 | 1.00 | 32.04 |
| | ATOM | 466 | CB | PHE | 367 | 17.138 | 6.291 | 10.016 | 1.00 | 30.22 |
| | ATOM | 467 | CG | PHE | 367 | 18.544 | 5.773 | 10.080 | 1.00 | 30.60 |
| 30 | ATOM | 468 | CD1 | PHE | 367 | 18.827 | 4.446 | 9.751 | 1.00 | 31.94 |
| | ATOM | 469 | CD2 | PHE | 367 | 19.589 | 6.601 | 10.485 | 1.00 | 29.20 |
| | ATOM | 470 | CE1 | PHE | 367 | 20.133 | 3.950 | 9.828 | 1.00 | 28.30 |
| | ATOM | 471 | CE2 | PHE | 367 | 20.896 | 6.122 | 10.568 | 1.00 | 28.12 |
| | ATOM | 472 | CZ | PHE | 367 | 21.171 | 4.791 | 10.240 | 1.00 | 25.41 |
| 35 | ATOM | 473 | C | PHE | 367 | 17.033 | 6.333 | 7.524 | 1.00 | 31.46 |
| | ATOM | 474 | O | PHE | 367 | 18.073 | 6.405 | 6.883 | 1.00 | 32.30 |
| | ATOM | 475 | N | VAL | 368 | 16.027 | 5.541 | 7.165 | 1.00 | 35.20 |
| | ATOM | 476 | CA | VAL | 368 | 16.123 | 4.718 | 5.959 | 1.00 | 38.98 |
| | ATOM | 477 | CB | VAL | 368 | 15.076 | 3.584 | 5.945 | 1.00 | 40.61 |
| 40 | ATOM | 478 | CG1 | VAL | 368 | 15.543 | 2.447 | 6.843 | 1.00 | 41.48 |
| | ATOM | 479 | CG2 | VAL | 368 | 13.717 | 4.113 | 6.390 | 1.00 | 41.60 |
| | ATOM | 480 | C | VAL | 368 | 15.965 | 5.523 | 4.673 | 1.00 | 40.06 |
| | ATOM | 481 | O | VAL | 368 | 16.156 | 4.992 | 3.579 | 1.00 | 41.66 |
| | ATOM | 482 | N | ASP | 369 | 15.608 | 6.798 | 4.798 | 1.00 | 38.65 |
| 45 | ATOM | 483 | CA | ASP | 369 | 15.465 | 7.646 | 3.621 | 1.00 | 37.15 |
| | ATOM | 484 | CB | ASP | 369 | 14.700 | 8.929 | 3.954 | 1.00 | 39.89 |
| | ATOM | 485 | CG | ASP | 369 | 13.254 | 8.671 | 4.302 | 1.00 | 45.59 |
| | ATOM | 486 | OD1 | ASP | 369 | 12.686 | 7.672 | 3.806 | 1.00 | 46.34 |
| | ATOM | 487 | OD2 | ASP | 369 | 12.681 | 9.472 | 5.074 | 1.00 | 49.13 |
| 50 | ATOM | 488 | C | ASP | 369 | 16.855 | 8.010 | 3.136 | 1.00 | 34.91 |
| | ATOM | 489 | O | ASP | 369 | 17.038 | 8.431 | 1.995 | 1.00 | 34.25 |
| | ATOM | 490 | N | LEU | 370 | 17.838 | 7.841 | 4.016 | 1.00 | 31.76 |
| | ATOM | 491 | CA | LEU | 370 | 19.229 | 8.153 | 3.705 | 1.00 | 28.08 |
| | ATOM | 492 | CB | LEU | 370 | 20.020 | 8.339 | 5.003 | 1.00 | 28.81 |
| 55 | ATOM | 493 | CG | LEU | 370 | 19.523 | 9.395 | 6.000 | 1.00 | 28.74 |
| | ATOM | 494 | CD1 | LEU | 370 | 20.315 | 9.275 | 7.299 | 1.00 | 30.81 |
| | ATOM | 495 | CD2 | LEU | 370 | 19.693 | 10.792 | 5.404 | 1.00 | 29.77 |
| | ATOM | 496 | C | LEU | 370 | 19.884 | 7.043 | 2.893 | 1.00 | 31.25 |
| | ATOM | 497 | O | LEU | 370 | 19.341 | 5.943 | 2.784 | 1.00 | 31.78 |
| 60 | ATOM | 498 | N | THR | 371 | 21.052 | 7.333 | 2.331 | 1.00 | 28.86 |
| | ATOM | 499 | CA | THR | 371 | 21.793 | 6.336 | 1.569 | 1.00 | 32.90 |

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|----|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 500 | CB | THR | 371 | 22.979 | 6.944 | 0.818 | 1.00 | 33.44 |
| | ATOM | 501 | OG1 | THR | 371 | 23.880 | 7.523 | 1.766 | 1.00 | 34.59 |
| | ATOM | 502 | CG2 | THR | 371 | 22.514 | 8.002 | -0.178 | 1.00 | 32.63 |
| | ATOM | 503 | C | THR | 371 | 22.373 | 5.315 | 2.539 | 1.00 | 35.31 |
| | ATOM | 504 | O | THR | 371 | 22.536 | 5.591 | 3.733 | 1.00 | 31.27 |
| 10 | ATOM | 505 | N | LEU | 372 | 22.702 | 4.141 | 2.015 | 1.00 | 34.34 |
| | ATOM | 506 | CA | LEU | 372 | 23.273 | 3.073 | 2.822 | 1.00 | 35.46 |
| | ATOM | 507 | CB | LEU | 372 | 23.518 | 1.841 | 1.944 | 1.00 | 37.73 |
| | ATOM | 508 | CG | LEU | 372 | 24.362 | 0.704 | 2.515 | 1.00 | 42.43 |
| | ATOM | 509 | CD1 | LEU | 372 | 23.690 | 0.145 | 3.757 | 1.00 | 45.60 |
| 15 | ATOM | 510 | CD2 | LEU | 372 | 24.534 | -0.383 | 1.455 | 1.00 | 44.29 |
| | ATOM | 511 | C | LEU | 372 | 24.587 | 3.548 | 3.444 | 1.00 | 36.95 |
| | ATOM | 512 | O | LEU | 372 | 24.813 | 3.374 | 4.643 | 1.00 | 35.57 |
| | ATOM | 513 | N | HIS | 373 | 25.442 | 4.159 | 2.627 | 1.00 | 35.68 |
| | ATOM | 514 | CA | HIS | 373 | 26.729 | 4.656 | 3.099 | 1.00 | 36.60 |
| 20 | ATOM | 515 | CB | HIS | 373 | 27.506 | 5.282 | 1.935 | 1.00 | 44.01 |
| | ATOM | 516 | CG | HIS | 373 | 28.538 | 6.280 | 2.360 | 1.00 | 50.69 |
| | ATOM | 517 | CD2 | HIS | 373 | 29.857 | 6.138 | 2.636 | 1.00 | 54.69 |
| | ATOM | 518 | ND1 | HIS | 373 | 28.246 | 7.613 | 2.561 | 1.00 | 53.77 |
| | ATOM | 519 | CE1 | HIS | 373 | 29.339 | 8.248 | 2.945 | 1.00 | 57.09 |
| 25 | ATOM | 520 | NE2 | HIS | 373 | 30.331 | 7.376 | 2.999 | 1.00 | 57.23 |
| | ATOM | 521 | C | HIS | 373 | 26.575 | 5.669 | 4.244 | 1.00 | 36.22 |
| | ATOM | 522 | O | HIS | 373 | 27.350 | 5.650 | 5.201 | 1.00 | 33.05 |
| | ATOM | 523 | N | ASP | 374 | 25.580 | 6.549 | 4.148 | 1.00 | 32.03 |
| | ATOM | 524 | CA | ASP | 374 | 25.342 | 7.541 | 5.196 | 1.00 | 30.76 |
| 30 | ATOM | 525 | CB | ASP | 374 | 24.354 | 8.603 | 4.713 | 1.00 | 30.12 |
| | ATOM | 526 | CG | ASP | 374 | 25.018 | 9.672 | 3.860 | 1.00 | 35.83 |
| | ATOM | 527 | OD1 | ASP | 374 | 26.264 | 9.744 | 3.842 | 1.00 | 34.39 |
| | ATOM | 528 | OD2 | ASP | 374 | 24.291 | 10.440 | 3.199 | 1.00 | 35.39 |
| | ATOM | 529 | C | ASP | 374 | 24.805 | 6.876 | 6.472 | 1.00 | 30.33 |
| 35 | ATOM | 530 | O | ASP | 374 | 25.152 | 7.275 | 7.587 | 1.00 | 27.04 |
| | ATOM | 531 | N | GLN | 375 | 23.944 | 5.877 | 6.309 | 1.00 | 25.71 |
| | ATOM | 532 | CA | GLN | 375 | 23.403 | 5.157 | 7.454 | 1.00 | 26.68 |
| | ATOM | 533 | CB | GLN | 375 | 22.424 | 4.077 | 6.993 | 1.00 | 29.70 |
| | ATOM | 534 | CG | GLN | 375 | 21.101 | 4.616 | 6.484 | 1.00 | 29.16 |
| 40 | ATOM | 535 | CD | GLN | 375 | 20.219 | 3.514 | 5.940 | 1.00 | 35.87 |
| | ATOM | 536 | OE1 | GLN | 375 | 20.155 | 2.426 | 6.510 | 1.00 | 30.97 |
| | ATOM | 537 | NE2 | GLN | 375 | 19.541 | 3.785 | 4.827 | 1.00 | 34.51 |
| | ATOM | 538 | C | GLN | 375 | 24.556 | 4.502 | 8.214 | 1.00 | 25.51 |
| | ATOM | 539 | O | GLN | 375 | 24.585 | 4.513 | 9.442 | 1.00 | 28.14 |
| 45 | ATOM | 540 | N | VAL | 376 | 25.504 | 3.938 | 7.475 | 1.00 | 26.62 |
| | ATOM | 541 | CA | VAL | 376 | 26.659 | 3.281 | 8.071 | 1.00 | 29.24 |
| | ATOM | 542 | CB | VAL | 376 | 27.531 | 2.597 | 7.003 | 1.00 | 29.66 |
| | ATOM | 543 | CG1 | VAL | 376 | 28.812 | 2.071 | 7.635 | 1.00 | 28.29 |
| | ATOM | 544 | CG2 | VAL | 376 | 26.745 | 1.469 | 6.341 | 1.00 | 29.90 |
| 50 | ATOM | 545 | C | VAL | 376 | 27.526 | 4.285 | 8.821 | 1.00 | 30.87 |
| | ATOM | 546 | O | VAL | 376 | 27.953 | 4.029 | 9.948 | 1.00 | 30.09 |
| | ATOM | 547 | N | HIS | 377 | 27.785 | 5.428 | 8.191 | 1.00 | 28.05 |
| | ATOM | 548 | CA | HIS | 377 | 28.602 | 6.457 | 8.814 | 1.00 | 28.68 |
| | ATOM | 549 | CB | HIS | 377 | 28.792 | 7.639 | 7.864 | 1.00 | 30.26 |
| 55 | ATOM | 550 | CG | HIS | 377 | 29.508 | 8.791 | 8.488 | 1.00 | 33.89 |
| | ATOM | 551 | CD2 | HIS | 377 | 29.073 | 10.017 | 8.863 | 1.00 | 34.99 |
| | ATOM | 552 | ND1 | HIS | 377 | 30.846 | 8.740 | 8.823 | 1.00 | 37.01 |
| | ATOM | 553 | CE1 | HIS | 377 | 31.201 | 9.884 | 9.377 | 1.00 | 34.79 |
| | ATOM | 554 | NE2 | HIS | 377 | 30.144 | 10.677 | 9.413 | 1.00 | 34.95 |
| 60 | ATOM | 555 | C | HIS | 377 | 27.983 | 6.954 | 10.114 | 1.00 | 25.13 |
| | ATOM | 556 | O | HIS | 377 | 28.677 | 7.102 | 11.115 | 1.00 | 25.93 |

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|----|------|-----|-----|------|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 557 | N | LEU | 378 | 26.678 | 7.206 | 10.107 | 1.00 | 24.58 |
| | ATOM | 558 | CA | LEU | 378 | 26.015 | 7.695 | 11.315 | 1.00 | 26.40 |
| | ATOM | 559 | CB | LEU | 378 | 24.542 | 8.001 | 11.027 | 1.00 | 26.29 |
| | ATOM | 560 | CG | LEU | 378 | 24.291 | 9.180 | 10.073 | 1.00 | 28.06 |
| 10 | ATOM | 561 | CD1 | LEU | 378 | 22.778 | 9.353 | 9.869 | 1.00 | 27.66 |
| | ATOM | 562 | CD2 | LEU | 378 | 24.911 | 10.458 | 10.642 | 1.00 | 30.08 |
| | ATOM | 563 | C | LEU | 378 | 26.120 | 6.695 | 12.459 | 1.00 | 28.55 |
| | ATOM | 564 | O | LEU | 378 | 26.379 | 7.075 | 13.605 | 1.00 | 24.76 |
| | ATOM | 565 | N | LEU | 379 | 25.919 | 5.414 | 12.153 | 1.00 | 24.29 |
| | ATOM | 566 | CA | LEU | 379 | 26.000 | 4.388 | 13.182 | 1.00 | 27.03 |
| 15 | ATOM | 567 | CB | LEU | 379 | 25.401 | 3.073 | 12.667 | 1.00 | 28.53 |
| | ATOM | 568 | CG | LEU | 379 | 23.875 | 3.023 | 12.845 | 1.00 | 30.29 |
| | ATOM | 569 | CD1 | LEU | 379 | 23.248 | 1.943 | 11.963 | 1.00 | 33.04 |
| | ATOM | 570 | CD2 | LEU | 379 | 23.563 | 2.759 | 14.312 | 1.00 | 29.45 |
| | ATOM | 571 | C | LEU | 379 | 27.430 | 4.176 | 13.670 | 1.00 | 27.18 |
| 20 | ATOM | 572 | O | LEU | 379 | 27.653 | 3.979 | 14.866 | 1.00 | 25.95 |
| | ATOM | 573 | N | GLU | 380 | 28.402 | 4.236 | 12.762 | 1.00 | 25.86 |
| | ATOM | 574 | CA | GLU | 380 | 29.786 | 4.054 | 13.173 | 1.00 | 27.58 |
| | ATOM | 575 | CB | GLU | 380 | 30.730 | 4.036 | 11.968 | 1.00 | 30.36 |
| | ATOM | 576 | CG | GLU | 380 | 32.172 | 3.785 | 12.380 | 1.00 | 37.98 |
| 25 | ATOM | 577 | CD | GLU | 380 | 33.080 | 3.471 | 11.210 | 1.00 | 45.23 |
| | ATOM | 578 | OE1 | GLU | 380 | 32.869 | 4.048 | 10.120 | 1.00 | 42.99 |
| | ATOM | 579 | OE2 | GLU | 380 | 34.004 | 2.646 | 11.386 | 1.00 | 45.79 |
| | ATOM | 580 | C | GLU | 380 | 30.218 | 5.159 | 14.133 | 1.00 | 27.50 |
| 30 | ATOM | 581 | O | GLU | 380 | 31.056 | 4.937 | 15.010 | 1.00 | 26.67 |
| | ATOM | 582 | N | ACYS | 381 | 29.637 | 6.339 | 13.965 | 0.75 | 24.89 |
| | ATOM | 583 | N | BCYS | 381 | 29.645 | 6.352 | 13.980 | 0.25 | 25.79 |
| | ATOM | 584 | CA | ACYS | 381 | 29.969 | 7.466 | 14.826 | 0.75 | 24.12 |
| | ATOM | 585 | CA | BCYS | 381 | 29.993 | 7.481 | 14.847 | 0.25 | 24.86 |
| 35 | ATOM | 586 | CB | ACYS | 381 | 29.621 | 8.781 | 14.122 | 0.75 | 25.96 |
| | ATOM | 587 | CB | BCYS | 381 | 29.766 | 8.814 | 14.115 | 0.25 | 25.62 |
| | ATOM | 588 | SG | ACYS | 381 | 30.698 | 9.192 | 12.732 | 0.75 | 31.63 |
| | ATOM | 589 | SG | BCYS | 381 | 30.227 | 10.312 | 15.059 | 0.25 | 25.40 |
| | ATOM | 590 | C | ACYS | 381 | 29.237 | 7.422 | 16.162 | 0.75 | 22.07 |
| | ATOM | 591 | C | BCYS | 381 | 29.211 | 7.498 | 16.159 | 0.25 | 23.97 |
| 40 | ATOM | 592 | O | ACYS | 381 | 29.812 | 7.730 | 17.206 | 0.75 | 21.97 |
| | ATOM | 593 | O | BCYS | 381 | 29.724 | 7.940 | 17.187 | 0.25 | 23.99 |
| | ATOM | 594 | N | ALA | 382 | 27.974 | 7.012 | 16.128 | 1.00 | 23.41 |
| | ATOM | 595 | CA | ALA | 382 | 27.140 | 7.015 | 17.318 | 1.00 | 22.83 |
| 45 | ATOM | 596 | CB | ALA | 382 | 25.785 | 7.587 | 16.948 | 1.00 | 25.50 |
| | ATOM | 597 | C | ALA | 382 | 26.913 | 5.755 | 18.131 | 1.00 | 25.39 |
| | ATOM | 598 | O | ALA | 382 | 26.374 | 5.837 | 19.234 | 1.00 | 23.09 |
| | ATOM | 599 | N | TRP | 383 | 27.311 | 4.602 | 17.615 | 1.00 | 25.98 |
| | ATOM | 600 | CA | TRP | 383 | 27.026 | 3.354 | 18.318 | 1.00 | 23.80 |
| 50 | ATOM | 601 | CB | TRP | 383 | 27.669 | 2.172 | 17.580 | 1.00 | 22.52 |
| | ATOM | 602 | CG | TRP | 383 | 29.130 | 2.054 | 17.762 | 1.00 | 24.42 |
| | ATOM | 603 | CD2 | TRP | 383 | 29.797 | 1.347 | 18.803 | 1.00 | 27.31 |
| | ATOM | 604 | CE2 | TRP | 383 | 31.182 | 1.484 | 18.579 | 1.00 | 28.24 |
| | ATOM | 605 | CE3 | TRP | 383 | 29.360 | 0.609 | 19.912 | 1.00 | 27.37 |
| 55 | ATOM | 606 | CD1 | TRP | 383 | 30.102 | 2.578 | 16.965 | 1.00 | 24.58 |
| | ATOM | 607 | NE1 | TRP | 383 | 31.342 | 2.239 | 17.446 | 1.00 | 27.35 |
| | ATOM | 608 | CZ2 | TRP | 383 | 32.133 | 0.909 | 19.420 | 1.00 | 28.76 |
| | ATOM | 609 | CZ3 | TRP | 383 | 30.305 | 0.039 | 20.745 | 1.00 | 28.09 |
| | ATOM | 610 | CH2 | TRP | 383 | 31.674 | 0.191 | 20.496 | 1.00 | 29.77 |
| 60 | ATOM | 611 | C | TRP | 383 | 27.356 | 3.309 | 19.802 | 1.00 | 23.54 |
| | ATOM | 612 | O | TRP | 383 | 26.526 | 2.866 | 20.584 | 1.00 | 22.90 |
| | ATOM | 613 | N | LEU | 384 | 28.542 | 3.765 | 20.211 | 1.00 | 20.37 |

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|----|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 614 | CA | LEU | 384 | 28.864 | 3.713 | 21.640 | 1.00 | 22.41 |
| | ATOM | 615 | CB | LEU | 384 | 30.369 | 3.890 | 21.883 | 1.00 | 24.98 |
| | ATOM | 616 | CG | LEU | 384 | 30.824 | 3.645 | 23.336 | 1.00 | 27.33 |
| | ATOM | 617 | CD1 | LEU | 384 | 30.273 | 2.305 | 23.853 | 1.00 | 29.71 |
| | ATOM | 618 | CD2 | LEU | 384 | 32.336 | 3.648 | 23.398 | 1.00 | 26.07 |
| 10 | ATOM | 619 | C | LEU | 384 | 28.075 | 4.732 | 22.453 | 1.00 | 19.44 |
| | ATOM | 620 | O | LEU | 384 | 27.706 | 4.458 | 23.595 | 1.00 | 23.24 |
| | ATOM | 621 | N | GLU | 385 | 27.807 | 5.909 | 21.885 | 1.00 | 20.80 |
| | ATOM | 622 | CA | GLU | 385 | 27.011 | 6.895 | 22.612 | 1.00 | 21.32 |
| | ATOM | 623 | CB | GLU | 385 | 26.861 | 8.177 | 21.797 | 1.00 | 21.91 |
| 15 | ATOM | 624 | CG | GLU | 385 | 28.115 | 9.020 | 21.705 | 1.00 | 21.61 |
| | ATOM | 625 | CD | GLU | 385 | 27.882 | 10.256 | 20.860 | 1.00 | 29.53 |
| | ATOM | 626 | OE1 | GLU | 385 | 27.374 | 11.256 | 21.401 | 1.00 | 30.54 |
| | ATOM | 627 | OE2 | GLU | 385 | 28.188 | 10.219 | 19.658 | 1.00 | 29.97 |
| | ATOM | 628 | C | GLU | 385 | 25.616 | 6.292 | 22.836 | 1.00 | 22.26 |
| 20 | ATOM | 629 | O | GLU | 385 | 25.022 | 6.438 | 23.902 | 1.00 | 22.26 |
| | ATOM | 630 | N | ILE | 386 | 25.101 | 5.617 | 21.812 | 1.00 | 22.03 |
| | ATOM | 631 | CA | ILE | 386 | 23.779 | 4.995 | 21.896 | 1.00 | 22.74 |
| | ATOM | 632 | CB | ILE | 386 | 23.328 | 4.455 | 20.498 | 1.00 | 22.88 |
| | ATOM | 633 | CG2 | ILE | 386 | 22.009 | 3.647 | 20.618 | 1.00 | 23.85 |
| 25 | ATOM | 634 | CG1 | ILE | 386 | 23.085 | 5.651 | 19.561 | 1.00 | 25.05 |
| | ATOM | 635 | CD1 | ILE | 386 | 22.994 | 5.297 | 18.078 | 1.00 | 26.42 |
| | ATOM | 636 | C | ILE | 386 | 23.766 | 3.897 | 22.961 | 1.00 | 22.50 |
| | ATOM | 637 | O | ILE | 386 | 22.823 | 3.818 | 23.746 | 1.00 | 24.75 |
| | ATOM | 638 | N | LEU | 387 | 24.810 | 3.071 | 23.020 | 1.00 | 22.25 |
| 30 | ATOM | 639 | CA | LEU | 387 | 24.868 | 2.030 | 24.051 | 1.00 | 22.95 |
| | ATOM | 640 | CB | LEU | 387 | 26.096 | 1.132 | 23.864 | 1.00 | 24.61 |
| | ATOM | 641 | CG | LEU | 387 | 26.070 | 0.194 | 22.654 | 1.00 | 23.21 |
| | ATOM | 642 | CD1 | LEU | 387 | 27.297 | -0.709 | 22.705 | 1.00 | 25.36 |
| | ATOM | 643 | CD2 | LEU | 387 | 24.791 | -0.631 | 22.652 | 1.00 | 26.29 |
| 35 | ATOM | 644 | C | LEU | 387 | 24.944 | 2.660 | 25.438 | 1.00 | 26.22 |
| | ATOM | 645 | O | LEU | 387 | 24.287 | 2.204 | 26.386 | 1.00 | 23.55 |
| | ATOM | 646 | N | MET | 388 | 25.751 | 3.713 | 25.554 | 1.00 | 23.92 |
| | ATOM | 647 | CA | MET | 388 | 25.924 | 4.385 | 26.835 | 1.00 | 24.26 |
| | ATOM | 648 | CB | MET | 388 | 27.088 | 5.378 | 26.761 | 1.00 | 23.87 |
| 40 | ATOM | 649 | CG | MET | 388 | 28.440 | 4.722 | 26.743 | 1.00 | 24.08 |
| | ATOM | 650 | SD | MET | 388 | 29.726 | 5.992 | 26.736 | 1.00 | 27.70 |
| | ATOM | 651 | CE | MET | 388 | 31.139 | 5.041 | 27.078 | 1.00 | 21.74 |
| | ATOM | 652 | C | MET | 388 | 24.660 | 5.094 | 27.321 | 1.00 | 23.33 |
| | ATOM | 653 | O | MET | 388 | 24.341 | 5.026 | 28.505 | 1.00 | 25.58 |
| 45 | ATOM | 654 | N | ILE | 389 | 23.935 | 5.775 | 26.436 | 1.00 | 24.62 |
| | ATOM | 655 | CA | ILE | 389 | 22.729 | 6.440 | 26.905 | 1.00 | 24.03 |
| | ATOM | 656 | CB | ILE | 389 | 22.132 | 7.439 | 25.852 | 1.00 | 27.01 |
| | ATOM | 657 | CG2 | ILE | 389 | 21.413 | 6.705 | 24.706 | 1.00 | 23.98 |
| | ATOM | 658 | CG1 | ILE | 389 | 21.185 | 8.402 | 26.584 | 1.00 | 25.49 |
| 50 | ATOM | 659 | CD1 | ILE | 389 | 20.431 | 9.383 | 25.683 | 1.00 | 25.45 |
| | ATOM | 660 | C | ILE | 389 | 21.694 | 5.401 | 27.349 | 1.00 | 26.54 |
| | ATOM | 661 | O | ILE | 389 | 20.938 | 5.631 | 28.294 | 1.00 | 22.58 |
| | ATOM | 662 | N | GLY | 390 | 21.679 | 4.247 | 26.687 | 1.00 | 27.14 |
| | ATOM | 663 | CA | GLY | 390 | 20.753 | 3.201 | 27.090 | 1.00 | 28.42 |
| 55 | ATOM | 664 | C | GLY | 390 | 21.133 | 2.719 | 28.482 | 1.00 | 29.67 |
| | ATOM | 665 | O | GLY | 390 | 20.275 | 2.521 | 29.348 | 1.00 | 29.21 |
| | ATOM | 666 | N | LEU | 391 | 22.433 | 2.547 | 28.699 | 1.00 | 26.06 |
| | ATOM | 667 | CA | LEU | 391 | 22.955 | 2.091 | 29.983 | 1.00 | 29.23 |
| | ATOM | 668 | CB | LEU | 391 | 24.476 | 1.937 | 29.899 | 1.00 | 28.37 |
| 60 | ATOM | 669 | CG | LEU | 391 | 25.206 | 1.656 | 31.210 | 1.00 | 30.81 |
| | ATOM | 670 | CD1 | LEU | 391 | 24.717 | 0.332 | 31.793 | 1.00 | 25.73 |

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|----|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 671 | CD2 | LEU | 391 | 26.709 | 1.619 | 30.958 | 1.00 | 25.25 |
| | ATOM | 672 | C | LEU | 391 | 22.603 | 3.070 | 31.104 | 1.00 | 30.84 |
| | ATOM | 673 | O | LEU | 391 | 22.156 | 2.669 | 32.186 | 1.00 | 29.19 |
| | ATOM | 674 | N | VAL | 392 | 22.817 | 4.355 | 30.850 | 1.00 | 28.91 |
| | ATOM | 675 | CA | VAL | 392 | 22.506 | 5.369 | 31.851 | 1.00 | 28.86 |
| 10 | ATOM | 676 | CB | VAL | 392 | 22.923 | 6.770 | 31.353 | 1.00 | 30.08 |
| | ATOM | 677 | CG1 | VAL | 392 | 22.329 | 7.854 | 32.237 | 1.00 | 32.32 |
| | ATOM | 678 | CG2 | VAL | 392 | 24.442 | 6.870 | 31.372 | 1.00 | 28.52 |
| | ATOM | 679 | C | VAL | 392 | 21.013 | 5.327 | 32.165 | 1.00 | 28.42 |
| | ATOM | 680 | O | VAL | 392 | 20.621 | 5.345 | 33.327 | 1.00 | 30.38 |
| 15 | ATOM | 681 | N | TRP | 393 | 20.191 | 5.241 | 31.125 | 1.00 | 28.23 |
| | ATOM | 682 | CA | TRP | 393 | 18.732 | 5.186 | 31.280 | 1.00 | 29.70 |
| | ATOM | 683 | CB | TRP | 393 | 18.066 | 5.046 | 29.906 | 1.00 | 30.09 |
| | ATOM | 684 | CG | TRP | 393 | 16.605 | 4.670 | 29.953 | 1.00 | 33.50 |
| | ATOM | 685 | CD2 | TRP | 393 | 15.516 | 5.499 | 30.369 | 1.00 | 31.76 |
| 20 | ATOM | 686 | CE2 | TRP | 393 | 14.336 | 4.725 | 30.264 | 1.00 | 38.11 |
| | ATOM | 687 | CE3 | TRP | 393 | 15.419 | 6.821 | 30.824 | 1.00 | 32.56 |
| | ATOM | 688 | CD1 | TRP | 393 | 16.057 | 3.459 | 29.618 | 1.00 | 34.31 |
| | ATOM | 689 | NE1 | TRP | 393 | 14.696 | 3.486 | 29.801 | 1.00 | 34.36 |
| | ATOM | 690 | CZ2 | TRP | 393 | 13.073 | 5.233 | 30.597 | 1.00 | 37.93 |
| 25 | ATOM | 691 | CZ3 | TRP | 393 | 14.162 | 7.326 | 31.155 | 1.00 | 35.24 |
| | ATOM | 692 | CH2 | TRP | 393 | 13.007 | 6.531 | 31.039 | 1.00 | 37.77 |
| | ATOM | 693 | C | TRP | 393 | 18.256 | 4.051 | 32.191 | 1.00 | 32.07 |
| | ATOM | 694 | O | TRP | 393 | 17.460 | 4.275 | 33.109 | 1.00 | 32.12 |
| | ATOM | 695 | N | ARG | 394 | 18.738 | 2.837 | 31.957 | 1.00 | 31.90 |
| 30 | ATOM | 696 | CA | ARG | 394 | 18.288 | 1.729 | 32.787 | 1.00 | 36.63 |
| | ATOM | 697 | CB | ARG | 394 | 18.492 | 0.389 | 32.065 | 1.00 | 36.41 |
| | ATOM | 698 | CG | ARG | 394 | 19.914 | 0.009 | 31.764 | 1.00 | 36.50 |
| | ATOM | 699 | CD | ARG | 394 | 19.929 | -1.132 | 30.748 | 1.00 | 36.34 |
| | ATOM | 700 | NE | ARG | 394 | 21.282 | -1.561 | 30.417 | 1.00 | 33.97 |
| 35 | ATOM | 701 | CZ | ARG | 394 | 21.864 | -1.350 | 29.239 | 1.00 | 31.61 |
| | ATOM | 702 | NH1 | ARG | 394 | 21.208 | -0.715 | 28.281 | 1.00 | 32.42 |
| | ATOM | 703 | NH2 | ARG | 394 | 23.098 | -1.784 | 29.022 | 1.00 | 29.81 |
| | ATOM | 704 | C | ARG | 394 | 18.911 | 1.697 | 34.180 | 1.00 | 36.69 |
| | ATOM | 705 | O | ARG | 394 | 18.445 | 0.966 | 35.048 | 1.00 | 37.07 |
| 40 | ATOM | 706 | N | SER | 395 | 19.954 | 2.492 | 34.395 | 1.00 | 33.63 |
| | ATOM | 707 | CA | SER | 395 | 20.603 | 2.564 | 35.701 | 1.00 | 35.69 |
| | ATOM | 708 | CB | SER | 395 | 22.112 | 2.784 | 35.540 | 1.00 | 32.94 |
| | ATOM | 709 | OG | SER | 395 | 22.696 | 1.811 | 34.688 | 1.00 | 32.37 |
| | ATOM | 710 | C | SER | 395 | 20.010 | 3.713 | 36.531 | 1.00 | 36.44 |
| 45 | ATOM | 711 | O | SER | 395 | 20.389 | 3.916 | 37.687 | 1.00 | 38.68 |
| | ATOM | 712 | N | MET | 396 | 19.076 | 4.449 | 35.937 | 1.00 | 36.46 |
| | ATOM | 713 | CA | MET | 396 | 18.431 | 5.588 | 36.589 | 1.00 | 43.08 |
| | ATOM | 714 | CB | MET | 396 | 17.275 | 6.104 | 35.725 | 1.00 | 43.87 |
| | ATOM | 715 | CG | MET | 396 | 17.481 | 7.507 | 35.176 | 1.00 | 46.18 |
| 50 | ATOM | 716 | SD | MET | 396 | 15.962 | 8.278 | 34.581 | 1.00 | 49.58 |
| | ATOM | 717 | CE | MET | 396 | 14.988 | 8.298 | 36.065 | 1.00 | 53.58 |
| | ATOM | 718 | C | MET | 396 | 17.906 | 5.303 | 37.992 | 1.00 | 46.18 |
| | ATOM | 719 | O | MET | 396 | 18.125 | 6.089 | 38.913 | 1.00 | 46.34 |
| | ATOM | 720 | N | GLU | 397 | 17.215 | 4.180 | 38.152 | 1.00 | 49.39 |
| 55 | ATOM | 721 | CA | GLU | 397 | 16.645 | 3.821 | 39.444 | 1.00 | 52.12 |
| | ATOM | 722 | CB | GLU | 397 | 15.296 | 3.130 | 39.246 | 1.00 | 55.34 |
| | ATOM | 723 | CG | GLU | 397 | 14.166 | 4.073 | 38.873 | 1.00 | 58.86 |
| | ATOM | 724 | CD | GLU | 397 | 13.195 | 3.448 | 37.891 | 1.00 | 63.28 |
| | ATOM | 725 | OE1 | GLU | 397 | 13.660 | 2.925 | 36.854 | 1.00 | 64.68 |
| 60 | ATOM | 726 | OE2 | GLU | 397 | 11.972 | 3.475 | 38.155 | 1.00 | 65.39 |
| | ATOM | 727 | C | GLU | 397 | 17.548 | 2.933 | 40.283 | 1.00 | 52.75 |

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|----|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 728 | O | GLU | 397 | 17.071 | 2.187 | 41.139 | 1.00 | 53.96 |
| | ATOM | 729 | N | HIS | 398 | 18.851 | 3.014 | 40.040 | 1.00 | 50.25 |
| | ATOM | 730 | CA | HIS | 398 | 19.813 | 2.220 | 40.792 | 1.00 | 49.34 |
| | ATOM | 731 | CB | HIS | 398 | 20.271 | 1.018 | 39.963 | 1.00 | 52.04 |
| | ATOM | 732 | CG | HIS | 398 | 19.187 | 0.017 | 39.721 | 1.00 | 53.95 |
| 10 | ATOM | 733 | CD2 | HIS | 398 | 18.750 | -1.022 | 40.472 | 1.00 | 53.92 |
| | ATOM | 734 | ND1 | HIS | 398 | 18.374 | 0.054 | 38.608 | 1.00 | 55.91 |
| | ATOM | 735 | CE1 | HIS | 398 | 17.482 | -0.917 | 38.685 | 1.00 | 55.53 |
| | ATOM | 736 | NE2 | HIS | 398 | 17.688 | -1.585 | 39.806 | 1.00 | 55.81 |
| | ATOM | 737 | C | HIS | 398 | 20.999 | 3.084 | 41.196 | 1.00 | 47.44 |
| 15 | ATOM | 738 | O | HIS | 398 | 22.121 | 2.887 | 40.730 | 1.00 | 44.91 |
| | ATOM | 739 | N | PRO | 399 | 20.755 | 4.049 | 42.096 | 1.00 | 46.45 |
| | ATOM | 740 | CD | PRO | 399 | 19.443 | 4.300 | 42.721 | 1.00 | 47.27 |
| | ATOM | 741 | CA | PRO | 399 | 21.785 | 4.968 | 42.586 | 1.00 | 45.35 |
| | ATOM | 742 | CB | PRO | 399 | 21.127 | 5.631 | 43.793 | 1.00 | 47.40 |
| 20 | ATOM | 743 | CG | PRO | 399 | 19.660 | 5.561 | 43.504 | 1.00 | 47.72 |
| | ATOM | 744 | C | PRO | 399 | 23.086 | 4.270 | 42.958 | 1.00 | 44.70 |
| | ATOM | 745 | O | PRO | 399 | 23.078 | 3.233 | 43.627 | 1.00 | 46.46 |
| | ATOM | 746 | N | GLY | 400 | 24.202 | 4.840 | 42.509 | 1.00 | 41.57 |
| | ATOM | 747 | CA | GLY | 400 | 25.506 | 4.281 | 42.813 | 1.00 | 39.84 |
| 25 | ATOM | 748 | C | GLY | 400 | 25.907 | 3.047 | 42.022 | 1.00 | 37.85 |
| | ATOM | 749 | O | GLY | 400 | 27.027 | 2.560 | 42.176 | 1.00 | 40.48 |
| | ATOM | 750 | N | LYS | 401 | 25.012 | 2.537 | 41.180 | 1.00 | 36.39 |
| | ATOM | 751 | CA | LYS | 401 | 25.315 | 1.344 | 40.390 | 1.00 | 34.47 |
| | ATOM | 752 | CB | LYS | 401 | 24.562 | 0.130 | 40.947 | 1.00 | 36.12 |
| 30 | ATOM | 753 | CG | LYS | 401 | 24.633 | -0.007 | 42.466 | 1.00 | 39.30 |
| | ATOM | 754 | CD | LYS | 401 | 24.288 | -1.429 | 42.903 | 1.00 | 44.38 |
| | ATOM | 755 | CE | LYS | 401 | 24.459 | -1.605 | 44.408 | 1.00 | 46.68 |
| | ATOM | 756 | NZ | LYS | 401 | 24.968 | -2.969 | 44.747 | 1.00 | 53.37 |
| | ATOM | 757 | C | LYS | 401 | 24.969 | 1.485 | 38.911 | 1.00 | 32.34 |
| 35 | ATOM | 758 | O | LYS | 401 | 24.141 | 2.308 | 38.531 | 1.00 | 31.16 |
| | ATOM | 759 | N | LEU | 402 | 25.612 | 0.663 | 38.086 | 1.00 | 28.52 |
| | ATOM | 760 | CA | LEU | 402 | 25.358 | 0.658 | 36.648 | 1.00 | 29.06 |
| | ATOM | 761 | CB | LEU | 402 | 26.661 | 0.847 | 35.867 | 1.00 | 29.26 |
| | ATOM | 762 | CG | LEU | 402 | 27.278 | 2.242 | 36.029 | 1.00 | 24.67 |
| 40 | ATOM | 763 | CD1 | LEU | 402 | 28.623 | 2.310 | 35.310 | 1.00 | 27.47 |
| | ATOM | 764 | CD2 | LEU | 402 | 26.312 | 3.277 | 35.482 | 1.00 | 24.93 |
| | ATOM | 765 | C | LEU | 402 | 24.755 | -0.686 | 36.292 | 1.00 | 30.43 |
| | ATOM | 766 | O | LEU | 402 | 25.367 | -1.727 | 36.535 | 1.00 | 31.36 |
| | ATOM | 767 | N | LEU | 403 | 23.552 | -0.658 | 35.735 | 1.00 | 31.07 |
| 45 | ATOM | 768 | CA | LEU | 403 | 22.873 | -1.880 | 35.335 | 1.00 | 32.96 |
| | ATOM | 769 | CB | LEU | 403 | 21.361 | -1.693 | 35.434 | 1.00 | 33.86 |
| | ATOM | 770 | CG | LEU | 403 | 20.551 | -2.991 | 35.415 | 1.00 | 39.29 |
| | ATOM | 771 | CD1 | LEU | 403 | 20.584 | -3.637 | 36.806 | 1.00 | 43.62 |
| | ATOM | 772 | CD2 | LEU | 403 | 19.128 | -2.689 | 34.998 | 1.00 | 41.32 |
| 50 | ATOM | 773 | C | LEU | 403 | 23.255 | -2.218 | 33.899 | 1.00 | 30.06 |
| | ATOM | 774 | O | LEU | 403 | 22.543 | -1.870 | 32.956 | 1.00 | 31.63 |
| | ATOM | 775 | N | PHE | 404 | 24.383 | -2.893 | 33.733 | 1.00 | 29.19 |
| | ATOM | 776 | CA | PHE | 404 | 24.834 | -3.256 | 32.403 | 1.00 | 28.93 |
| | ATOM | 777 | CB | PHE | 404 | 26.201 | -3.929 | 32.493 | 1.00 | 30.05 |
| 55 | ATOM | 778 | CG | PHE | 404 | 27.305 | -2.998 | 32.926 | 1.00 | 30.78 |
| | ATOM | 779 | CD1 | PHE | 404 | 27.794 | -3.033 | 34.228 | 1.00 | 32.91 |
| | ATOM | 780 | CD2 | PHE | 404 | 27.848 | -2.078 | 32.030 | 1.00 | 32.75 |
| | ATOM | 781 | CE1 | PHE | 404 | 28.816 | -2.160 | 34.638 | 1.00 | 34.73 |
| | ATOM | 782 | CE2 | PHE | 404 | 28.864 | -1.205 | 32.423 | 1.00 | 30.68 |
| 60 | ATOM | 783 | CZ | PHE | 404 | 29.350 | -1.242 | 33.727 | 1.00 | 31.43 |
| | ATOM | 784 | C | PHE | 404 | 23.809 | -4.181 | 31.756 | 1.00 | 30.80 |

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|----|------|-----|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 785 | O | PHE | 404 | 23.625 | -4.175 | 30.538 | 1.00 | 28.09 |
| | ATOM | 786 | N | ALA | 405 | 23.138 | -4.967 | 32.594 | 1.00 | 30.25 |
| | ATOM | 787 | CA | ALA | 405 | 22.104 | -5.910 | 32.163 | 1.00 | 29.78 |
| | ATOM | 788 | CB | ALA | 405 | 22.745 | -7.172 | 31.598 | 1.00 | 29.97 |
| | ATOM | 789 | C | ALA | 405 | 21.309 | -6.237 | 33.429 | 1.00 | 31.95 |
| 10 | ATOM | 790 | O | ALA | 405 | 21.785 | -5.995 | 34.535 | 1.00 | 32.36 |
| | ATOM | 791 | N | PRO | 406 | 20.088 | -6.779 | 33.288 | 1.00 | 34.40 |
| | ATOM | 792 | CD | PRO | 406 | 19.356 | -7.102 | 32.053 | 1.00 | 35.81 |
| | ATOM | 793 | CA | PRO | 406 | 19.303 | -7.101 | 34.490 | 1.00 | 36.41 |
| | ATOM | 794 | CB | PRO | 406 | 17.985 | -7.654 | 33.935 | 1.00 | 35.38 |
| 15 | ATOM | 795 | CG | PRO | 406 | 17.922 | -7.153 | 32.519 | 1.00 | 36.49 |
| | ATOM | 796 | C | PRO | 406 | 19.997 | -8.084 | 35.433 | 1.00 | 37.32 |
| | ATOM | 797 | O | PRO | 406 | 19.698 | -8.112 | 36.626 | 1.00 | 38.34 |
| | ATOM | 798 | N | ASN | 407 | 20.924 | -8.877 | 34.902 | 1.00 | 36.69 |
| | ATOM | 799 | CA | ASN | 407 | 21.652 | -9.847 | 35.712 | 1.00 | 38.85 |
| 20 | ATOM | 800 | CB | ASN | 407 | 21.582 | -11.243 | 35.083 | 1.00 | 39.69 |
| | ATOM | 801 | CG | ASN | 407 | 22.232 | -11.306 | 33.711 | 1.00 | 44.10 |
| | ATOM | 802 | OD1 | ASN | 407 | 22.345 | -10.296 | 33.009 | 1.00 | 37.78 |
| | ATOM | 803 | ND2 | ASN | 407 | 22.660 | -12.503 | 33.319 | 1.00 | 45.74 |
| | ATOM | 804 | C | ASN | 407 | 23.100 | -9.435 | 35.874 | 1.00 | 38.12 |
| 25 | ATOM | 805 | O | ASN | 407 | 23.965 | -10.256 | 36.178 | 1.00 | 39.81 |
| | ATOM | 806 | N | LEU | 408 | 23.364 | -8.149 | 35.671 | 1.00 | 37.80 |
| | ATOM | 807 | CA | LEU | 408 | 24.713 | -7.631 | 35.799 | 1.00 | 36.89 |
| | ATOM | 808 | CB | LEU | 408 | 25.449 | -7.720 | 34.459 | 1.00 | 36.09 |
| | ATOM | 809 | CG | LEU | 408 | 26.972 | -7.609 | 34.550 | 1.00 | 35.08 |
| 30 | ATOM | 810 | CD1 | LEU | 408 | 27.525 | -8.775 | 35.354 | 1.00 | 39.15 |
| | ATOM | 811 | CD2 | LEU | 408 | 27.578 | -7.587 | 33.158 | 1.00 | 36.85 |
| | ATOM | 812 | C | LEU | 408 | 24.670 | -6.187 | 36.286 | 1.00 | 40.55 |
| | ATOM | 813 | O | LEU | 408 | 24.646 | -5.248 | 35.491 | 1.00 | 38.29 |
| | ATOM | 814 | N | LEU | 409 | 24.644 | -6.034 | 37.607 | 1.00 | 39.50 |
| 35 | ATOM | 815 | CA | LEU | 409 | 24.606 | -4.733 | 38.257 | 1.00 | 41.00 |
| | ATOM | 816 | CB | LEU | 409 | 23.392 | -4.658 | 39.184 | 1.00 | 43.69 |
| | ATOM | 817 | CG | LEU | 409 | 23.164 | -3.382 | 39.993 | 1.00 | 47.35 |
| | ATOM | 818 | CD1 | LEU | 409 | 22.848 | -2.233 | 39.058 | 1.00 | 47.09 |
| | ATOM | 819 | CD2 | LEU | 409 | 22.014 | -3.603 | 40.976 | 1.00 | 49.38 |
| 40 | ATOM | 820 | C | LEU | 409 | 25.894 | -4.566 | 39.060 | 1.00 | 41.80 |
| | ATOM | 821 | O | LEU | 409 | 26.178 | -5.358 | 39.960 | 1.00 | 41.00 |
| | ATOM | 822 | N | LEU | 410 | 26.676 | -3.544 | 38.727 | 1.00 | 39.23 |
| | ATOM | 823 | CA | LEU | 410 | 27.931 | -3.296 | 39.423 | 1.00 | 40.45 |
| | ATOM | 824 | CB | LEU | 410 | 29.106 | -3.354 | 38.442 | 1.00 | 41.59 |
| 45 | ATOM | 825 | CG | LEU | 410 | 29.457 | -4.660 | 37.716 | 1.00 | 44.87 |
| | ATOM | 826 | CD1 | LEU | 410 | 30.972 | -4.728 | 37.554 | 1.00 | 45.41 |
| | ATOM | 827 | CD2 | LEU | 410 | 28.949 | -5.872 | 38.484 | 1.00 | 47.02 |
| | ATOM | 828 | C | LEU | 410 | 27.946 | -1.944 | 40.132 | 1.00 | 40.67 |
| | ATOM | 829 | O | LEU | 410 | 27.361 | -0.970 | 39.652 | 1.00 | 40.22 |
| 50 | ATOM | 830 | N | ASP | 411 | 28.610 | -1.890 | 41.281 | 1.00 | 41.57 |
| | ATOM | 831 | CA | ASP | 411 | 28.717 | -0.640 | 42.025 | 1.00 | 42.69 |
| | ATOM | 832 | CB | ASP | 411 | 28.490 | -0.874 | 43.528 | 1.00 | 44.44 |
| | ATOM | 833 | CG | ASP | 411 | 29.655 | -1.578 | 44.210 | 1.00 | 46.70 |
| | ATOM | 834 | OD1 | ASP | 411 | 29.537 | -1.849 | 45.426 | 1.00 | 51.44 |
| 55 | ATOM | 835 | OD2 | ASP | 411 | 30.680 | -1.861 | 43.553 | 1.00 | 48.79 |
| | ATOM | 836 | C | ASP | 411 | 30.088 | -0.016 | 41.779 | 1.00 | 43.70 |
| | ATOM | 837 | O | ASP | 411 | 30.933 | -0.610 | 41.107 | 1.00 | 38.48 |
| | ATOM | 838 | N | ARG | 412 | 30.295 | 1.181 | 42.321 | 1.00 | 46.78 |
| | ATOM | 839 | CA | ARG | 412 | 31.554 | 1.905 | 42.171 | 1.00 | 49.97 |
| 60 | ATOM | 840 | CB | ARG | 412 | 31.601 | 3.090 | 43.138 | 1.00 | 51.28 |
| | ATOM | 841 | CG | ARG | 412 | 30.971 | 4.364 | 42.614 | 1.00 | 54.77 |

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|----|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 842 | CD | ARG | 412 | 31.644 | 5.580 | 43.219 | 1.00 | 54.61 |
| | ATOM | 843 | NE | ARG | 412 | 33.071 | 5.615 | 42.912 | 1.00 | 56.53 |
| | ATOM | 844 | CZ | ARG | 412 | 33.827 | 6.708 | 42.985 | 1.00 | 61.90 |
| | ATOM | 845 | NH1 | ARG | 412 | 33.291 | 7.866 | 43.356 | 1.00 | 63.48 |
| | ATOM | 846 | NH2 | ARG | 412 | 35.120 | 6.645 | 42.682 | 1.00 | 61.21 |
| 10 | ATOM | 847 | C | ARG | 412 | 32.771 | 1.026 | 42.429 | 1.00 | 50.29 |
| | ATOM | 848 | O | ARG | 412 | 33.628 | 0.866 | 41.561 | 1.00 | 51.02 |
| | ATOM | 849 | N | ASN | 413 | 32.844 | 0.469 | 43.633 | 1.00 | 51.94 |
| | ATOM | 850 | CA | ASN | 413 | 33.969 | -0.375 | 44.021 | 1.00 | 53.15 |
| | ATOM | 851 | CB | ASN | 413 | 33.719 | -0.980 | 45.403 | 1.00 | 55.88 |
| 15 | ATOM | 852 | CG | ASN | 413 | 33.654 | 0.073 | 46.496 | 1.00 | 57.99 |
| | ATOM | 853 | OD1 | ASN | 413 | 33.697 | 1.276 | 46.223 | 1.00 | 58.27 |
| | ATOM | 854 | ND2 | ASN | 413 | 33.551 | -0.375 | 47.742 | 1.00 | 57.90 |
| | ATOM | 855 | C | ASN | 413 | 34.235 | -1.480 | 43.013 | 1.00 | 53.95 |
| | ATOM | 856 | O | ASN | 413 | 35.386 | -1.743 | 42.659 | 1.00 | 53.67 |
| 20 | ATOM | 857 | N | GLN | 414 | 33.173 | -2.129 | 42.547 | 1.00 | 55.33 |
| | ATOM | 858 | CA | GLN | 414 | 33.326 | -3.198 | 41.573 | 1.00 | 55.42 |
| | ATOM | 859 | CB | GLN | 414 | 31.991 | -3.904 | 41.343 | 1.00 | 55.44 |
| | ATOM | 860 | CG | GLN | 414 | 31.645 | -4.933 | 42.391 | 1.00 | 56.07 |
| | ATOM | 861 | CD | GLN | 414 | 30.203 | -5.376 | 42.336 | 1.00 | 57.40 |
| 25 | ATOM | 862 | OE1 | GLN | 414 | 29.296 | -4.536 | 42.402 | 1.00 | 60.22 |
| | ATOM | 863 | NE2 | GLN | 414 | 29.973 | -6.664 | 42.199 | 1.00 | 57.27 |
| | ATOM | 864 | C | GLN | 414 | 33.850 | -2.630 | 40.259 | 1.00 | 55.51 |
| | ATOM | 865 | O | GLN | 414 | 34.654 | -3.265 | 39.578 | 1.00 | 56.16 |
| | ATOM | 866 | N | GLY | 415 | 33.398 | -1.430 | 39.910 | 1.00 | 57.07 |
| 30 | ATOM | 867 | CA | GLY | 415 | 33.849 | -0.806 | 38.680 | 1.00 | 58.51 |
| | ATOM | 868 | C | GLY | 415 | 35.350 | -0.582 | 38.689 | 1.00 | 61.10 |
| | ATOM | 869 | O | GLY | 415 | 36.023 | -0.748 | 37.671 | 1.00 | 59.47 |
| | ATOM | 870 | N | LYS | 416 | 35.877 | -0.211 | 39.851 | 1.00 | 62.77 |
| | ATOM | 871 | CA | LYS | 416 | 37.305 | 0.041 | 40.011 | 1.00 | 65.49 |
| 35 | ATOM | 872 | CB | LYS | 416 | 37.634 | 0.262 | 41.491 | 1.00 | 66.04 |
| | ATOM | 873 | CG | LYS | 416 | 38.121 | 1.663 | 41.823 | 1.00 | 68.71 |
| | ATOM | 874 | CD | LYS | 416 | 37.078 | 2.439 | 42.613 | 1.00 | 70.98 |
| | ATOM | 875 | CE | LYS | 416 | 37.404 | 2.448 | 44.100 | 1.00 | 71.84 |
| | ATOM | 876 | NZ | LYS | 416 | 36.225 | 2.079 | 44.933 | 1.00 | 71.95 |
| 40 | ATOM | 877 | C | LYS | 416 | 38.159 | -1.105 | 39.472 | 1.00 | 66.41 |
| | ATOM | 878 | O | LYS | 416 | 39.361 | -0.946 | 39.269 | 1.00 | 67.15 |
| | ATOM | 879 | N | CYS | 417 | 37.538 | -2.257 | 39.238 | 1.00 | 67.33 |
| | ATOM | 880 | CA | CYS | 417 | 38.270 | -3.414 | 38.741 | 1.00 | 68.16 |
| | ATOM | 881 | CB | CYS | 417 | 37.951 | -4.642 | 39.602 | 1.00 | 70.88 |
| 45 | ATOM | 882 | SG | CYS | 417 | 38.592 | -4.549 | 41.301 | 1.00 | 76.09 |
| | ATOM | 883 | C | CYS | 417 | 38.015 | -3.736 | 37.270 | 1.00 | 67.54 |
| | ATOM | 884 | O | CYS | 417 | 38.632 | -4.653 | 36.720 | 1.00 | 68.48 |
| | ATOM | 885 | N | VAL | 418 | 37.111 | -2.994 | 36.631 | 1.00 | 64.67 |
| | ATOM | 886 | CA | VAL | 418 | 36.817 | -3.226 | 35.218 | 1.00 | 59.97 |
| 50 | ATOM | 887 | CB | VAL | 418 | 35.326 | -2.917 | 34.879 | 1.00 | 59.60 |
| | ATOM | 888 | CG1 | VAL | 418 | 34.971 | -1.503 | 35.284 | 1.00 | 59.13 |
| | ATOM | 889 | CG2 | VAL | 418 | 35.072 | -3.121 | 33.391 | 1.00 | 54.85 |
| | ATOM | 890 | C | VAL | 418 | 37.739 | -2.362 | 34.355 | 1.00 | 58.37 |
| | ATOM | 891 | O | VAL | 418 | 37.799 | -1.140 | 34.512 | 1.00 | 55.44 |
| 55 | ATOM | 892 | N | GLU | 419 | 38.463 | -3.012 | 33.450 | 1.00 | 56.02 |
| | ATOM | 893 | CA | GLU | 419 | 39.403 | -2.328 | 32.570 | 1.00 | 54.28 |
| | ATOM | 894 | CB | GLU | 419 | 40.149 | -3.351 | 31.710 | 1.00 | 57.57 |
| | ATOM | 895 | CG | GLU | 419 | 39.385 | -3.779 | 30.468 | 1.00 | 60.87 |
| | ATOM | 896 | CD | GLU | 419 | 40.179 | -4.722 | 29.584 | 1.00 | 63.34 |
| 60 | ATOM | 897 | OE1 | GLU | 419 | 40.432 | -5.870 | 30.011 | 1.00 | 64.90 |
| | ATOM | 898 | OE2 | GLU | 419 | 40.546 | -4.313 | 28.462 | 1.00 | 63.18 |

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|----|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 899 | C | GLU | 419 | 38.761 | -1.281 | 31.662 | 1.00 | 52.05 |
| | ATOM | 900 | O | GLU | 419 | 37.665 | -1.481 | 31.131 | 1.00 | 49.82 |
| | ATOM | 901 | N | GLY | 420 | 39.465 | -0.165 | 31.491 | 1.00 | 49.45 |
| | ATOM | 902 | CA | GLY | 420 | 38.983 | 0.908 | 30.642 | 1.00 | 46.22 |
| | ATOM | 903 | C | GLY | 420 | 37.895 | 1.767 | 31.254 | 1.00 | 44.55 |
| 10 | ATOM | 904 | O | GLY | 420 | 37.417 | 2.705 | 30.619 | 1.00 | 42.08 |
| | ATOM | 905 | N | MET | 421 | 37.503 | 1.471 | 32.488 | 1.00 | 43.41 |
| | ATOM | 906 | CA | MET | 421 | 36.449 | 2.248 | 33.123 | 1.00 | 42.48 |
| | ATOM | 907 | CB | MET | 421 | 35.306 | 1.327 | 33.554 | 1.00 | 42.34 |
| | ATOM | 908 | CG | MET | 421 | 34.590 | 0.635 | 32.396 | 1.00 | 38.22 |
| 15 | ATOM | 909 | SD | MET | 421 | 32.927 | 0.102 | 32.843 | 1.00 | 38.56 |
| | ATOM | 910 | CE | MET | 421 | 32.003 | 1.699 | 32.766 | 1.00 | 35.54 |
| | ATOM | 911 | C | MET | 421 | 36.923 | 3.059 | 34.312 | 1.00 | 41.64 |
| | ATOM | 912 | O | MET | 421 | 36.113 | 3.512 | 35.111 | 1.00 | 39.77 |
| | ATOM | 913 | N | VAL | 422 | 38.232 | 3.256 | 34.430 | 1.00 | 43.42 |
| 20 | ATOM | 914 | CA | VAL | 422 | 38.757 | 4.019 | 35.557 | 1.00 | 44.79 |
| | ATOM | 915 | CB | VAL | 422 | 40.285 | 4.248 | 35.433 | 1.00 | 46.54 |
| | ATOM | 916 | CG1 | VAL | 422 | 40.595 | 5.086 | 34.206 | 1.00 | 48.25 |
| | ATOM | 917 | CG2 | VAL | 422 | 40.813 | 4.920 | 36.696 | 1.00 | 46.24 |
| | ATOM | 918 | C | VAL | 422 | 38.056 | 5.372 | 35.689 | 1.00 | 44.09 |
| 25 | ATOM | 919 | O | VAL | 422 | 37.691 | 5.783 | 36.783 | 1.00 | 44.12 |
| | ATOM | 920 | N | GLU | 423 | 37.846 | 6.055 | 34.570 | 1.00 | 42.07 |
| | ATOM | 921 | CA | GLU | 423 | 37.192 | 7.356 | 34.616 | 1.00 | 40.24 |
| | ATOM | 922 | CB | GLU | 423 | 37.909 | 8.338 | 33.684 | 1.00 | 44.02 |
| | ATOM | 923 | CG | GLU | 423 | 39.411 | 8.467 | 33.893 | 1.00 | 50.04 |
| 30 | ATOM | 924 | CD | GLU | 423 | 40.096 | 9.158 | 32.719 | 1.00 | 55.64 |
| | ATOM | 925 | OE1 | GLU | 423 | 39.539 | 10.156 | 32.205 | 1.00 | 56.66 |
| | ATOM | 926 | OE2 | GLU | 423 | 41.188 | 8.703 | 32.306 | 1.00 | 58.02 |
| | ATOM | 927 | C | GLU | 423 | 35.704 | 7.337 | 34.250 | 1.00 | 35.77 |
| | ATOM | 928 | O | GLU | 423 | 34.881 | 7.955 | 34.919 | 1.00 | 33.20 |
| 35 | ATOM | 929 | N | ILE | 424 | 35.345 | 6.617 | 33.197 | 1.00 | 36.16 |
| | ATOM | 930 | CA | ILE | 424 | 33.949 | 6.643 | 32.771 | 1.00 | 31.63 |
| | ATOM | 931 | CB | ILE | 424 | 33.803 | 6.087 | 31.347 | 1.00 | 33.58 |
| | ATOM | 932 | CG2 | ILE | 424 | 34.639 | 6.936 | 30.395 | 1.00 | 33.48 |
| | ATOM | 933 | CG1 | ILE | 424 | 34.204 | 4.617 | 31.296 | 1.00 | 34.46 |
| 40 | ATOM | 934 | CD1 | ILE | 424 | 33.857 | 3.955 | 29.978 | 1.00 | 34.67 |
| | ATOM | 935 | C | ILE | 424 | 32.890 | 6.035 | 33.685 | 1.00 | 28.89 |
| | ATOM | 936 | O | ILE | 424 | 31.729 | 6.443 | 33.632 | 1.00 | 26.49 |
| | ATOM | 937 | N | PHE | 425 | 33.261 | 5.091 | 34.542 | 1.00 | 29.26 |
| | ATOM | 938 | CA | PHE | 425 | 32.257 | 4.520 | 35.447 | 1.00 | 29.87 |
| 45 | ATOM | 939 | CB | PHE | 425 | 32.903 | 3.529 | 36.423 | 1.00 | 31.26 |
| | ATOM | 940 | CG | PHE | 425 | 31.948 | 2.496 | 36.959 | 1.00 | 32.17 |
| | ATOM | 941 | CD1 | PHE | 425 | 31.124 | 2.783 | 38.048 | 1.00 | 33.70 |
| | ATOM | 942 | CD2 | PHE | 425 | 31.881 | 1.230 | 36.381 | 1.00 | 30.64 |
| | ATOM | 943 | CE1 | PHE | 425 | 30.244 | 1.814 | 38.563 | 1.00 | 32.60 |
| 50 | ATOM | 944 | CE2 | PHE | 425 | 31.010 | 0.256 | 36.881 | 1.00 | 31.55 |
| | ATOM | 945 | CZ | PHE | 425 | 30.189 | 0.549 | 37.973 | 1.00 | 33.34 |
| | ATOM | 946 | C | PHE | 425 | 31.594 | 5.649 | 36.240 | 1.00 | 30.17 |
| | ATOM | 947 | O | PHE | 425 | 30.368 | 5.774 | 36.276 | 1.00 | 26.71 |
| | ATOM | 948 | N | ASP | 426 | 32.415 | 6.483 | 36.870 | 1.00 | 29.45 |
| 55 | ATOM | 949 | CA | ASP | 426 | 31.893 | 7.587 | 37.661 | 1.00 | 32.29 |
| | ATOM | 950 | CB | ASP | 426 | 33.031 | 8.291 | 38.401 | 1.00 | 33.49 |
| | ATOM | 951 | CG | ASP | 426 | 33.455 | 7.546 | 39.655 | 1.00 | 39.42 |
| | ATOM | 952 | OD1 | ASP | 426 | 32.767 | 6.574 | 40.038 | 1.00 | 38.35 |
| | ATOM | 953 | OD2 | ASP | 426 | 34.480 | 7.934 | 40.256 | 1.00 | 39.58 |
| 60 | ATOM | 954 | C | ASP | 426 | 31.133 | 8.592 | 36.806 | 1.00 | 29.02 |
| | ATOM | 955 | O | ASP | 426 | 30.154 | 9.175 | 37.257 | 1.00 | 31.34 |

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|----|------|------|-----|------|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 956 | N | MET | 427 | 31.585 | 8.797 | 35.572 | 1.00 | 30.69 |
| | ATOM | 957 | CA | MET | 427 | 30.919 | 9.736 | 34.675 | 1.00 | 28.63 |
| | ATOM | 958 | CB | MET | 427 | 31.744 | 9.912 | 33.407 | 1.00 | 26.83 |
| | ATOM | 959 | CG | MET | 427 | 33.032 | 10.680 | 33.608 | 1.00 | 31.41 |
| | ATOM | 960 | SD | MET | 427 | 33.962 | 10.783 | 32.077 | 1.00 | 34.87 |
| 10 | ATOM | 961 | CE | MET | 427 | 35.409 | 11.753 | 32.643 | 1.00 | 44.60 |
| | ATOM | 962 | C | MET | 427 | 29.526 | 9.202 | 34.324 | 1.00 | 28.70 |
| | ATOM | 963 | O | MET | 427 | 28.536 | 9.947 | 34.302 | 1.00 | 25.01 |
| | ATOM | 964 | N | LEU | 428 | 29.451 | 7.902 | 34.057 | 1.00 | 25.13 |
| | ATOM | 965 | CA | LEU | 428 | 28.173 | 7.292 | 33.730 | 1.00 | 27.60 |
| 15 | ATOM | 966 | CB | LEU | 428 | 28.379 | 5.824 | 33.332 | 1.00 | 28.00 |
| | ATOM | 967 | CG | LEU | 428 | 29.039 | 5.682 | 31.957 | 1.00 | 26.99 |
| | ATOM | 968 | CD1 | LEU | 428 | 29.678 | 4.303 | 31.782 | 1.00 | 27.80 |
| | ATOM | 969 | CD2 | LEU | 428 | 27.995 | 5.927 | 30.894 | 1.00 | 25.33 |
| | ATOM | 970 | C | LEU | 428 | 27.210 | 7.412 | 34.916 | 1.00 | 29.59 |
| 20 | ATOM | 971 | O | LEU | 428 | 26.041 | 7.743 | 34.743 | 1.00 | 27.07 |
| | ATOM | 972 | N | LEU | 429 | 27.701 | 7.147 | 36.126 | 1.00 | 30.40 |
| | ATOM | 973 | CA | LEU | 429 | 26.859 | 7.251 | 37.323 | 1.00 | 30.59 |
| | ATOM | 974 | CB | LEU | 429 | 27.675 | 6.884 | 38.571 | 1.00 | 31.76 |
| | ATOM | 975 | CG | LEU | 429 | 28.078 | 5.415 | 38.757 | 1.00 | 32.43 |
| 25 | ATOM | 976 | CD1 | LEU | 429 | 28.961 | 5.264 | 39.995 | 1.00 | 31.60 |
| | ATOM | 977 | CD2 | LEU | 429 | 26.825 | 4.573 | 38.903 | 1.00 | 34.66 |
| | ATOM | 978 | C | LEU | 429 | 26.319 | 8.681 | 37.466 | 1.00 | 30.46 |
| | ATOM | 979 | O | LEU | 429 | 25.143 | 8.901 | 37.769 | 1.00 | 28.40 |
| | ATOM | 980 | N | ALA | 430 | 27.193 | 9.656 | 37.237 | 1.00 | 31.34 |
| 30 | ATOM | 981 | CA | ALA | 430 | 26.806 | 11.059 | 37.332 | 1.00 | 29.83 |
| | ATOM | 982 | CB | ALA | 430 | 28.017 | 11.951 | 37.078 | 1.00 | 31.29 |
| | ATOM | 983 | C | ALA | 430 | 25.696 | 11.387 | 36.344 | 1.00 | 31.04 |
| | ATOM | 984 | O | ALA | 430 | 24.753 | 12.107 | 36.674 | 1.00 | 30.79 |
| | ATOM | 985 | N | THR | 431 | 25.802 | 10.854 | 35.128 | 1.00 | 30.30 |
| 35 | ATOM | 986 | CA | THR | 431 | 24.786 | 11.105 | 34.112 | 1.00 | 28.81 |
| | ATOM | 987 | CB | THR | 431 | 25.207 | 10.533 | 32.737 | 1.00 | 30.55 |
| | ATOM | 988 | OG1 | THR | 431 | 26.569 | 10.893 | 32.465 | 1.00 | 31.88 |
| | ATOM | 989 | CG2 | THR | 431 | 24.321 | 11.087 | 31.634 | 1.00 | 25.63 |
| | ATOM | 990 | C | THR | 431 | 23.462 | 10.481 | 34.530 | 1.00 | 29.49 |
| 40 | ATOM | 991 | O | THR | 431 | 22.402 | 11.099 | 34.397 | 1.00 | 26.18 |
| | ATOM | 992 | N | SER | 432 | 23.520 | 9.253 | 35.037 | 1.00 | 28.11 |
| | ATOM | 993 | CA | SER | 432 | 22.308 | 8.573 | 35.480 | 1.00 | 29.78 |
| | ATOM | 994 | CB | SER | 432 | 22.639 | 7.177 | 36.008 | 1.00 | 33.11 |
| | ATOM | 995 | OG | SER | 432 | 21.454 | 6.412 | 36.136 | 1.00 | 36.92 |
| 45 | ATOM | 996 | C | SER | 432 | 21.651 | 9.399 | 36.589 | 1.00 | 31.49 |
| | ATOM | 997 | O | SER | 432 | 20.433 | 9.576 | 36.613 | 1.00 | 30.09 |
| | ATOM | 998 | N | ASER | 433 | 22.476 | 9.901 | 37.496 | 0.75 | 32.09 |
| | ATOM | 999 | N | BSER | 433 | 22.474 | 9.906 | 37.500 | 0.25 | 31.10 |
| | ATOM | 1000 | CA | ASER | 433 | 22.002 | 10.715 | 38.605 | 0.75 | 35.68 |
| 50 | ATOM | 1001 | CA | BSER | 433 | 21.985 | 10.717 | 38.608 | 0.25 | 32.21 |
| | ATOM | 1002 | CB | ASER | 433 | 23.185 | 11.097 | 39.502 | 0.75 | 37.18 |
| | ATOM | 1003 | CB | BSER | 433 | 23.145 | 11.104 | 39.529 | 0.25 | 31.45 |
| | ATOM | 1004 | OG | ASER | 433 | 22.823 | 12.090 | 40.443 | 0.75 | 44.09 |
| | ATOM | 1005 | OG | BSER | 433 | 23.785 | 9.953 | 40.053 | 0.25 | 29.52 |
| 55 | ATOM | 1006 | C | ASER | 433 | 21.299 | 11.971 | 38.091 | 0.75 | 35.01 |
| | ATOM | 1007 | C | BSER | 433 | 21.295 | 11.976 | 38.092 | 0.25 | 32.88 |
| | ATOM | 1008 | O | ASER | 433 | 20.257 | 12.373 | 38.612 | 0.75 | 35.34 |
| | ATOM | 1009 | O | BSER | 433 | 20.264 | 12.391 | 38.622 | 0.25 | 33.42 |
| | ATOM | 1010 | N | ARG | 434 | 21.867 | 12.579 | 37.054 | 1.00 | 33.38 |
| 60 | ATOM | 1011 | CA | ARG | 434 | 21.300 | 13.788 | 36.470 | 1.00 | 34.19 |
| | ATOM | 1012 | CB | ARG | 434 | 22.239 | 14.354 | 35.400 | 1.00 | 33.89 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1013 | CG | ARG | 434 | 21.670 | 15.528 | 34.625 | 1.00 | 38.30 |
| | ATOM | 1014 | CD | ARG | 434 | 21.559 | 16.787 | 35.479 | 1.00 | 37.91 |
| | ATOM | 1015 | NE | ARG | 434 | 21.158 | 17.944 | 34.680 | 1.00 | 37.78 |
| | ATOM | 1016 | CZ | ARG | 434 | 20.488 | 18.995 | 35.149 | 1.00 | 41.06 |
| | ATOM | 1017 | NH1 | ARG | 434 | 20.132 | 19.049 | 36.428 | 1.00 | 40.70 |
| 10 | ATOM | 1018 | NH2 | ARG | 434 | 20.175 | 19.998 | 34.337 | 1.00 | 38.78 |
| | ATOM | 1019 | C | ARG | 434 | 19.937 | 13.491 | 35.873 | 1.00 | 33.48 |
| | ATOM | 1020 | O | ARG | 434 | 18.996 | 14.266 | 36.053 | 1.00 | 30.54 |
| | ATOM | 1021 | N | PHE | 435 | 19.831 | 12.371 | 35.158 | 1.00 | 34.68 |
| | ATOM | 1022 | CA | PHE | 435 | 18.563 | 11.963 | 34.549 | 1.00 | 35.02 |
| 15 | ATOM | 1023 | CB | PHE | 435 | 18.727 | 10.634 | 33.796 | 1.00 | 34.96 |
| | ATOM | 1024 | CG | PHE | 435 | 19.240 | 10.779 | 32.386 | 1.00 | 37.63 |
| | ATOM | 1025 | CD1 | PHE | 435 | 19.459 | 12.035 | 31.824 | 1.00 | 42.03 |
| | ATOM | 1026 | CD2 | PHE | 435 | 19.521 | 9.649 | 31.623 | 1.00 | 41.24 |
| | ATOM | 1027 | CE1 | PHE | 435 | 19.953 | 12.164 | 30.521 | 1.00 | 43.11 |
| 20 | ATOM | 1028 | CE2 | PHE | 435 | 20.016 | 9.768 | 30.322 | 1.00 | 40.59 |
| | ATOM | 1029 | CZ | PHE | 435 | 20.233 | 11.029 | 29.775 | 1.00 | 40.63 |
| | ATOM | 1030 | C | PHE | 435 | 17.527 | 11.780 | 35.657 | 1.00 | 35.49 |
| | ATOM | 1031 | O | PHE | 435 | 16.361 | 12.135 | 35.496 | 1.00 | 34.78 |
| | ATOM | 1032 | N | ARG | 436 | 17.968 | 11.216 | 36.777 | 1.00 | 38.27 |
| 25 | ATOM | 1033 | CA | ARG | 436 | 17.094 | 10.982 | 37.924 | 1.00 | 40.67 |
| | ATOM | 1034 | CB | ARG | 436 | 17.844 | 10.215 | 39.012 | 1.00 | 40.70 |
| | ATOM | 1035 | CG | ARG | 436 | 16.942 | 9.590 | 40.068 | 1.00 | 44.98 |
| | ATOM | 1036 | CD | ARG | 436 | 17.648 | 8.459 | 40.810 | 1.00 | 48.09 |
| | ATOM | 1037 | NE | ARG | 436 | 18.982 | 8.841 | 41.275 | 1.00 | 50.16 |
| 30 | ATOM | 1038 | CZ | ARG | 436 | 20.119 | 8.361 | 40.777 | 1.00 | 52.19 |
| | ATOM | 1039 | NH1 | ARG | 436 | 20.099 | 7.472 | 39.790 | 1.00 | 49.34 |
| | ATOM | 1040 | NH2 | ARG | 436 | 21.283 | 8.770 | 41.266 | 1.00 | 51.85 |
| | ATOM | 1041 | C | ARG | 436 | 16.576 | 12.302 | 38.493 | 1.00 | 40.40 |
| | ATOM | 1042 | O | ARG | 436 | 15.382 | 12.458 | 38.730 | 1.00 | 41.49 |
| 35 | ATOM | 1043 | N | MET | 437 | 17.477 | 13.252 | 38.706 | 1.00 | 40.02 |
| | ATOM | 1044 | CA | MET | 437 | 17.090 | 14.546 | 39.245 | 1.00 | 41.02 |
| | ATOM | 1045 | CB | MET | 437 | 18.329 | 15.427 | 39.440 | 1.00 | 40.29 |
| | ATOM | 1046 | C | MET | 437 | 16.099 | 15.221 | 38.299 | 1.00 | 40.81 |
| | ATOM | 1047 | O | MET | 437 | 15.111 | 15.805 | 38.734 | 1.00 | 42.46 |
| 40 | ATOM | 1048 | N | MET | 438 | 16.367 | 15.127 | 37.001 | 1.00 | 39.02 |
| | ATOM | 1049 | CA | MET | 438 | 15.510 | 15.732 | 35.988 | 1.00 | 40.11 |
| | ATOM | 1050 | CB | MET | 438 | 16.237 | 15.793 | 34.651 | 1.00 | 38.16 |
| | ATOM | 1051 | CG | MET | 438 | 17.352 | 16.794 | 34.601 | 1.00 | 41.52 |
| | ATOM | 1052 | SD | MET | 438 | 17.999 | 16.862 | 32.943 | 1.00 | 43.94 |
| 45 | ATOM | 1053 | CE | MET | 438 | 16.698 | 17.748 | 32.096 | 1.00 | 39.96 |
| | ATOM | 1054 | C | MET | 438 | 14.221 | 14.964 | 35.783 | 1.00 | 37.72 |
| | ATOM | 1055 | O | MET | 438 | 13.305 | 15.451 | 35.125 | 1.00 | 36.82 |
| | ATOM | 1056 | N | ASN | 439 | 14.155 | 13.759 | 36.337 | 1.00 | 38.81 |
| | ATOM | 1057 | CA | ASN | 439 | 12.981 | 12.919 | 36.174 | 1.00 | 40.77 |
| 50 | ATOM | 1058 | CB | ASN | 439 | 11.762 | 13.556 | 36.847 | 1.00 | 44.52 |
| | ATOM | 1059 | CG | ASN | 439 | 10.566 | 12.620 | 36.887 | 1.00 | 48.29 |
| | ATOM | 1060 | OD1 | ASN | 439 | 10.721 | 11.400 | 36.964 | 1.00 | 48.48 |
| | ATOM | 1061 | ND2 | ASN | 439 | 9.365 | 13.189 | 36.829 | 1.00 | 50.23 |
| | ATOM | 1062 | C | ASN | 439 | 12.725 | 12.744 | 34.677 | 1.00 | 39.36 |
| 55 | ATOM | 1063 | O | ASN | 439 | 11.637 | 13.037 | 34.172 | 1.00 | 37.76 |
| | ATOM | 1064 | N | LEU | 440 | 13.749 | 12.274 | 33.972 | 1.00 | 37.65 |
| | ATOM | 1065 | CA | LEU | 440 | 13.655 | 12.052 | 32.532 | 1.00 | 35.22 |
| | ATOM | 1066 | CB | LEU | 440 | 14.999 | 11.576 | 31.987 | 1.00 | 34.70 |
| | ATOM | 1067 | CG | LEU | 440 | 15.022 | 11.467 | 30.462 | 1.00 | 35.45 |
| 60 | ATOM | 1068 | CD1 | LEU | 440 | 14.890 | 12.862 | 29.869 | 1.00 | 35.24 |
| | ATOM | 1069 | CD2 | LEU | 440 | 16.297 | 10.795 | 29.999 | 1.00 | 35.30 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1070 | C | LEU | 440 | 12.587 | 11.024 | 32.196 | 1.00 | 36.48 |
| | ATOM | 1071 | O | LEU | 440 | 12.518 | 9.967 | 32.826 | 1.00 | 37.36 |
| | ATOM | 1072 | N | GLN | 441 | 11.763 | 11.328 | 31.197 | 1.00 | 36.82 |
| | ATOM | 1073 | CA | GLN | 441 | 10.696 | 10.420 | 30.785 | 1.00 | 38.51 |
| | ATOM | 1074 | CB | GLN | 441 | 9.431 | 11.211 | 30.443 | 1.00 | 38.23 |
| 10 | ATOM | 1075 | CG | GLN | 441 | 8.912 | 12.063 | 31.592 | 1.00 | 42.46 |
| | ATOM | 1076 | CD | GLN | 441 | 8.362 | 11.227 | 32.729 | 1.00 | 44.91 |
| | ATOM | 1077 | OE1 | GLN | 441 | 7.268 | 10.668 | 32.629 | 1.00 | 47.31 |
| | ATOM | 1078 | NE2 | GLN | 441 | 9.119 | 11.132 | 33.818 | 1.00 | 44.06 |
| | ATOM | 1079 | C | GLN | 441 | 11.099 | 9.565 | 29.585 | 1.00 | 38.48 |
| 15 | ATOM | 1080 | O | GLN | 441 | 11.923 | 9.976 | 28.763 | 1.00 | 35.80 |
| | ATOM | 1081 | N | GLY | 442 | 10.500 | 8.378 | 29.494 | 1.00 | 36.03 |
| | ATOM | 1082 | CA | GLY | 442 | 10.792 | 7.468 | 28.401 | 1.00 | 37.72 |
| | ATOM | 1083 | C | GLY | 442 | 10.599 | 8.112 | 27.043 | 1.00 | 36.88 |
| | ATOM | 1084 | O | GLY | 442 | 11.381 | 7.877 | 26.123 | 1.00 | 33.72 |
| 20 | ATOM | 1085 | N | GLU | 443 | 9.556 | 8.925 | 26.918 | 1.00 | 36.59 |
| | ATOM | 1086 | CA | GLU | 443 | 9.269 | 9.603 | 25.661 | 1.00 | 37.13 |
| | ATOM | 1087 | CB | GLU | 443 | 7.956 | 10.379 | 25.764 | 1.00 | 41.57 |
| | ATOM | 1088 | CG | GLU | 443 | 6.723 | 9.488 | 25.879 | 1.00 | 47.76 |
| | ATOM | 1089 | CD | GLU | 443 | 6.483 | 9.008 | 27.302 | 1.00 | 53.96 |
| 25 | ATOM | 1090 | OE1 | GLU | 443 | 5.619 | 8.123 | 27.498 | 1.00 | 57.66 |
| | ATOM | 1091 | OE2 | GLU | 443 | 7.159 | 9.515 | 28.225 | 1.00 | 56.13 |
| | ATOM | 1092 | C | GLU | 443 | 10.408 | 10.551 | 25.311 | 1.00 | 35.27 |
| | ATOM | 1093 | O | GLU | 443 | 10.759 | 10.704 | 24.145 | 1.00 | 33.85 |
| | ATOM | 1094 | N | GLU | 444 | 10.984 | 11.179 | 26.331 | 1.00 | 32.09 |
| 30 | ATOM | 1095 | CA | GLU | 444 | 12.097 | 12.095 | 26.126 | 1.00 | 33.92 |
| | ATOM | 1096 | CB | GLU | 444 | 12.332 | 12.924 | 27.388 | 1.00 | 34.97 |
| | ATOM | 1097 | CG | GLU | 444 | 11.169 | 13.845 | 27.732 | 1.00 | 38.28 |
| | ATOM | 1098 | CD | GLU | 444 | 11.383 | 14.610 | 29.023 | 1.00 | 38.11 |
| | ATOM | 1099 | OE1 | GLU | 444 | 11.800 | 13.993 | 30.026 | 1.00 | 39.53 |
| 35 | ATOM | 1100 | OE2 | GLU | 444 | 11.132 | 15.834 | 29.036 | 1.00 | 40.77 |
| | ATOM | 1101 | C | GLU | 444 | 13.356 | 11.305 | 25.770 | 1.00 | 33.59 |
| | ATOM | 1102 | O | GLU | 444 | 14.085 | 11.670 | 24.842 | 1.00 | 33.35 |
| | ATOM | 1103 | N | PHE | 445 | 13.590 | 10.215 | 26.501 | 1.00 | 30.68 |
| | ATOM | 1104 | CA | PHE | 445 | 14.753 | 9.357 | 26.276 | 1.00 | 32.49 |
| 40 | ATOM | 1105 | CB | PHE | 445 | 14.703 | 8.139 | 27.203 | 1.00 | 29.35 |
| | ATOM | 1106 | CG | PHE | 445 | 15.667 | 7.047 | 26.828 | 1.00 | 30.78 |
| | ATOM | 1107 | CD1 | PHE | 445 | 17.036 | 7.201 | 27.030 | 1.00 | 28.25 |
| | ATOM | 1108 | CD2 | PHE | 445 | 15.205 | 5.863 | 26.266 | 1.00 | 30.62 |
| | ATOM | 1109 | CE1 | PHE | 445 | 17.933 | 6.195 | 26.675 | 1.00 | 28.67 |
| 45 | ATOM | 1110 | CE2 | PHE | 445 | 16.095 | 4.848 | 25.908 | 1.00 | 31.37 |
| | ATOM | 1111 | CZ | PHE | 445 | 17.460 | 5.015 | 26.113 | 1.00 | 30.37 |
| | ATOM | 1112 | C | PHE | 445 | 14.850 | 8.885 | 24.829 | 1.00 | 31.11 |
| | ATOM | 1113 | O | PHE | 445 | 15.924 | 8.947 | 24.221 | 1.00 | 32.20 |
| | ATOM | 1114 | N | VAL | 446 | 13.739 | 8.415 | 24.266 | 1.00 | 28.63 |
| 50 | ATOM | 1115 | CA | VAL | 446 | 13.787 | 7.943 | 22.889 | 1.00 | 27.94 |
| | ATOM | 1116 | CB | VAL | 446 | 12.478 | 7.193 | 22.478 | 1.00 | 28.48 |
| | ATOM | 1117 | CG1 | VAL | 446 | 12.318 | 5.939 | 23.343 | 1.00 | 29.61 |
| | ATOM | 1118 | CG2 | VAL | 446 | 11.265 | 8.092 | 22.607 | 1.00 | 27.23 |
| | ATOM | 1119 | C | VAL | 446 | 14.099 | 9.064 | 21.900 | 1.00 | 27.28 |
| 55 | ATOM | 1120 | O | VAL | 446 | 14.781 | 8.837 | 20.904 | 1.00 | 28.07 |
| | ATOM | 1121 | N | CYS | 447 | 13.619 | 10.275 | 22.166 | 1.00 | 28.97 |
| | ATOM | 1122 | CA | CYS | 447 | 13.919 | 11.394 | 21.272 | 1.00 | 29.14 |
| | ATOM | 1123 | CB | CYS | 447 | 13.156 | 12.653 | 21.693 | 1.00 | 28.90 |
| | ATOM | 1124 | SG | CYS | 447 | 11.389 | 12.591 | 21.309 | 1.00 | 35.68 |
| 60 | ATOM | 1125 | C | CYS | 447 | 15.420 | 11.677 | 21.328 | 1.00 | 28.03 |
| | ATOM | 1126 | O | CYS | 447 | 16.063 | 11.885 | 20.302 | 1.00 | 29.34 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1127 | N | LEU | 448 | 15.969 | 11.686 | 22.538 | 1.00 | 27.28 |
| | ATOM | 1128 | CA | LEU | 448 | 17.392 | 11.938 | 22.729 | 1.00 | 25.30 |
| | ATOM | 1129 | CB | LEU | 448 | 17.733 | 11.932 | 24.220 | 1.00 | 27.72 |
| | ATOM | 1130 | CG | LEU | 448 | 17.248 | 13.135 | 25.040 | 1.00 | 29.54 |
| | ATOM | 1131 | CD1 | LEU | 448 | 17.807 | 13.042 | 26.454 | 1.00 | 30.85 |
| 10 | ATOM | 1132 | CD2 | LEU | 448 | 17.688 | 14.434 | 24.376 | 1.00 | 30.24 |
| | ATOM | 1133 | C | LEU | 448 | 18.245 | 10.902 | 22.008 | 1.00 | 27.62 |
| | ATOM | 1134 | O | LEU | 448 | 19.207 | 11.252 | 21.327 | 1.00 | 25.10 |
| | ATOM | 1135 | N | LYS | 449 | 17.905 | 9.621 | 22.162 | 1.00 | 25.16 |
| | ATOM | 1136 | CA | LYS | 449 | 18.673 | 8.570 | 21.506 | 1.00 | 27.55 |
| 15 | ATOM | 1137 | CB | LYS | 449 | 18.135 | 7.185 | 21.900 | 1.00 | 28.99 |
| | ATOM | 1138 | CG | LYS | 449 | 19.134 | 6.052 | 21.694 | 1.00 | 34.70 |
| | ATOM | 1139 | CD | LYS | 449 | 18.737 | 4.789 | 22.459 | 1.00 | 32.67 |
| | ATOM | 1140 | CE | LYS | 449 | 17.267 | 4.419 | 22.220 | 1.00 | 31.87 |
| | ATOM | 1141 | NZ | LYS | 449 | 17.022 | 2.967 | 22.472 | 1.00 | 29.14 |
| 20 | ATOM | 1142 | C | LYS | 449 | 18.626 | 8.749 | 19.990 | 1.00 | 25.88 |
| | ATOM | 1143 | O | LYS | 449 | 19.610 | 8.489 | 19.296 | 1.00 | 25.93 |
| | ATOM | 1144 | N | SER | 450 | 17.482 | 9.197 | 19.480 | 1.00 | 26.07 |
| | ATOM | 1145 | CA | SER | 450 | 17.323 | 9.421 | 18.052 | 1.00 | 27.24 |
| | ATOM | 1146 | CB | SER | 450 | 15.857 | 9.705 | 17.721 | 1.00 | 32.24 |
| 25 | ATOM | 1147 | OG | SER | 450 | 15.098 | 8.519 | 17.779 | 1.00 | 34.94 |
| | ATOM | 1148 | C | SER | 450 | 18.176 | 10.607 | 17.618 | 1.00 | 26.78 |
| | ATOM | 1149 | O | SER | 450 | 18.763 | 10.598 | 16.535 | 1.00 | 25.85 |
| | ATOM | 1150 | N | ILE | 451 | 18.231 | 11.632 | 18.463 | 1.00 | 26.94 |
| | ATOM | 1151 | CA | ILE | 451 | 19.032 | 12.810 | 18.155 | 1.00 | 26.13 |
| 30 | ATOM | 1152 | CB | ILE | 451 | 18.950 | 13.850 | 19.291 | 1.00 | 27.72 |
| | ATOM | 1153 | CG2 | ILE | 451 | 20.019 | 14.929 | 19.101 | 1.00 | 20.53 |
| | ATOM | 1154 | CG1 | ILE | 451 | 17.553 | 14.475 | 19.322 | 1.00 | 29.49 |
| | ATOM | 1155 | CD1 | ILE | 451 | 17.377 | 15.473 | 20.447 | 1.00 | 36.24 |
| | ATOM | 1156 | C | ILE | 451 | 20.489 | 12.381 | 17.989 | 1.00 | 24.88 |
| 35 | ATOM | 1157 | O | ILE | 451 | 21.161 | 12.771 | 17.034 | 1.00 | 26.96 |
| | ATOM | 1158 | N | ILE | 452 | 20.977 | 11.582 | 18.931 | 1.00 | 22.72 |
| | ATOM | 1159 | CA | ILE | 452 | 22.359 | 11.120 | 18.880 | 1.00 | 21.95 |
| | ATOM | 1160 | CB | ILE | 452 | 22.660 | 10.155 | 20.050 | 1.00 | 23.57 |
| | ATOM | 1161 | CG2 | ILE | 452 | 23.982 | 9.435 | 19.804 | 1.00 | 22.10 |
| 40 | ATOM | 1162 | CG1 | ILE | 452 | 22.718 | 10.949 | 21.371 | 1.00 | 21.70 |
| | ATOM | 1163 | CD1 | ILE | 452 | 22.768 | 10.060 | 22.624 | 1.00 | 25.30 |
| | ATOM | 1164 | C | ILE | 452 | 22.656 | 10.419 | 17.557 | 1.00 | 23.02 |
| | ATOM | 1165 | O | ILE | 452 | 23.650 | 10.708 | 16.885 | 1.00 | 21.25 |
| | ATOM | 1166 | N | LEU | 453 | 21.779 | 9.497 | 17.173 | 1.00 | 22.83 |
| 45 | ATOM | 1167 | CA | LEU | 453 | 21.984 | 8.768 | 15.935 | 1.00 | 22.05 |
| | ATOM | 1168 | CB | LEU | 453 | 20.843 | 7.764 | 15.733 | 1.00 | 22.06 |
| | ATOM | 1169 | CG | LEU | 453 | 20.712 | 7.189 | 14.324 | 1.00 | 22.03 |
| | ATOM | 1170 | CD1 | LEU | 453 | 21.815 | 6.165 | 14.107 | 1.00 | 24.81 |
| | ATOM | 1171 | CD2 | LEU | 453 | 19.328 | 6.535 | 14.156 | 1.00 | 24.73 |
| 50 | ATOM | 1172 | C | LEU | 453 | 22.092 | 9.687 | 14.717 | 1.00 | 23.95 |
| | ATOM | 1173 | O | LEU | 453 | 22.962 | 9.501 | 13.860 | 1.00 | 24.60 |
| | ATOM | 1174 | N | LEU | 454 | 21.220 | 10.687 | 14.638 | 1.00 | 26.72 |
| | ATOM | 1175 | CA | LEU | 454 | 21.234 | 11.599 | 13.494 | 1.00 | 26.45 |
| | ATOM | 1176 | CB | LEU | 454 | 19.852 | 12.242 | 13.330 | 1.00 | 25.51 |
| 55 | ATOM | 1177 | CG | LEU | 454 | 18.737 | 11.222 | 13.052 | 1.00 | 30.16 |
| | ATOM | 1178 | CD1 | LEU | 454 | 17.405 | 11.926 | 12.955 | 1.00 | 28.76 |
| | ATOM | 1179 | CD2 | LEU | 454 | 19.037 | 10.478 | 11.759 | 1.00 | 32.59 |
| | ATOM | 1180 | C | LEU | 454 | 22.292 | 12.703 | 13.552 | 1.00 | 28.24 |
| | ATOM | 1181 | O | LEU | 454 | 22.778 | 13.148 | 12.513 | 1.00 | 29.06 |
| 60 | ATOM | 1182 | N | ASN | 455 | 22.638 | 13.146 | 14.757 | 1.00 | 26.56 |
| | ATOM | 1183 | CA | ASN | 455 | 23.604 | 14.236 | 14.934 | 1.00 | 26.79 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1184 | CB | ASN | 455 | 23.284 | 14.998 | 16.224 | 1.00 | 26.20 |
| | ATOM | 1185 | CG | ASN | 455 | 24.174 | 16.217 | 16.419 | 1.00 | 27.26 |
| | ATOM | 1186 | OD1 | ASN | 455 | 24.171 | 17.134 | 15.602 | 1.00 | 30.83 |
| | ATOM | 1187 | ND2 | ASN | 455 | 24.931 | 16.230 | 17.506 | 1.00 | 27.16 |
| | ATOM | 1188 | C | ASN | 455 | 25.062 | 13.782 | 14.954 | 1.00 | 30.63 |
| 10 | ATOM | 1189 | O | ASN | 455 | 25.965 | 14.517 | 14.525 | 1.00 | 27.69 |
| | ATOM | 1190 | N | SER | 456 | 25.268 | 12.569 | 15.461 | 1.00 | 30.48 |
| | ATOM | 1191 | CA | SER | 456 | 26.572 | 11.928 | 15.579 | 1.00 | 35.26 |
| | ATOM | 1192 | CB | SER | 456 | 26.393 | 10.393 | 15.505 | 1.00 | 39.69 |
| | ATOM | 1193 | OG | SER | 456 | 25.871 | 9.953 | 14.243 | 1.00 | 30.73 |
| 15 | ATOM | 1194 | C | SER | 456 | 27.627 | 12.344 | 14.562 | 1.00 | 35.56 |
| | ATOM | 1195 | O | SER | 456 | 28.599 | 13.041 | 14.884 | 1.00 | 33.00 |
| | ATOM | 1196 | N | GLY | 457 | 27.437 | 11.886 | 13.334 | 1.00 | 33.88 |
| | ATOM | 1197 | CA | GLY | 457 | 28.393 | 12.189 | 12.292 | 1.00 | 36.77 |
| | ATOM | 1198 | C | GLY | 457 | 27.876 | 13.017 | 11.136 | 1.00 | 37.02 |
| 20 | ATOM | 1199 | O | GLY | 457 | 28.310 | 12.805 | 10.013 | 1.00 | 38.66 |
| | ATOM | 1200 | N | VAL | 458 | 26.967 | 13.956 | 11.392 | 1.00 | 39.12 |
| | ATOM | 1201 | CA | VAL | 458 | 26.438 | 14.802 | 10.317 | 1.00 | 43.81 |
| | ATOM | 1202 | CB | VAL | 458 | 25.231 | 15.648 | 10.755 | 1.00 | 44.25 |
| | ATOM | 1203 | CG1 | VAL | 458 | 24.209 | 15.713 | 9.631 | 1.00 | 44.51 |
| 25 | ATOM | 1204 | CG2 | VAL | 458 | 24.638 | 15.098 | 12.013 | 1.00 | 50.53 |
| | ATOM | 1205 | C | VAL | 458 | 27.472 | 15.801 | 9.817 | 1.00 | 46.72 |
| | ATOM | 1206 | O | VAL | 458 | 27.391 | 16.265 | 8.681 | 1.00 | 47.08 |
| | ATOM | 1207 | N | TYR | 459 | 28.432 | 16.144 | 10.670 | 1.00 | 50.74 |
| | ATOM | 1208 | CA | TYR | 459 | 29.456 | 17.114 | 10.301 | 1.00 | 55.43 |
| 30 | ATOM | 1209 | CB | TYR | 459 | 29.647 | 18.129 | 11.433 | 1.00 | 56.62 |
| | ATOM | 1210 | CG | TYR | 459 | 28.375 | 18.870 | 11.781 | 1.00 | 59.34 |
| | ATOM | 1211 | CD1 | TYR | 459 | 28.094 | 19.229 | 13.095 | 1.00 | 60.73 |
| | ATOM | 1212 | CE1 | TYR | 459 | 26.900 | 19.867 | 13.429 | 1.00 | 62.14 |
| | ATOM | 1213 | CD2 | TYR | 459 | 27.430 | 19.175 | 10.795 | 1.00 | 62.16 |
| 35 | ATOM | 1214 | CE2 | TYR | 459 | 26.234 | 19.812 | 11.118 | 1.00 | 63.83 |
| | ATOM | 1215 | CZ | TYR | 459 | 25.976 | 20.154 | 12.437 | 1.00 | 62.88 |
| | ATOM | 1216 | OH | TYR | 459 | 24.790 | 20.764 | 12.767 | 1.00 | 62.56 |
| | ATOM | 1217 | C | TYR | 459 | 30.791 | 16.489 | 9.928 | 1.00 | 57.21 |
| | ATOM | 1218 | O | TYR | 459 | 31.793 | 17.189 | 9.798 | 1.00 | 56.86 |
| 40 | ATOM | 1219 | N | THR | 460 | 30.800 | 15.173 | 9.750 | 1.00 | 59.22 |
| | ATOM | 1220 | CA | THR | 460 | 32.018 | 14.474 | 9.366 | 1.00 | 62.25 |
| | ATOM | 1221 | CB | THR | 460 | 32.502 | 13.531 | 10.499 | 1.00 | 63.07 |
| | ATOM | 1222 | OG1 | THR | 460 | 33.474 | 12.613 | 9.983 | 1.00 | 67.80 |
| | ATOM | 1223 | CG2 | THR | 460 | 31.344 | 12.759 | 11.084 | 1.00 | 60.23 |
| 45 | ATOM | 1224 | C | THR | 460 | 31.759 | 13.678 | 8.086 | 1.00 | 63.54 |
| | ATOM | 1225 | O | THR | 460 | 32.457 | 12.708 | 7.782 | 1.00 | 63.91 |
| | ATOM | 1226 | N | PHE | 461 | 30.758 | 14.113 | 7.326 | 1.00 | 65.06 |
| | ATOM | 1227 | CA | PHE | 461 | 30.395 | 13.446 | 6.080 | 1.00 | 67.00 |
| | ATOM | 1228 | CB | PHE | 461 | 29.052 | 13.975 | 5.563 | 1.00 | 66.48 |
| 50 | ATOM | 1229 | CG | PHE | 461 | 27.867 | 13.147 | 5.991 | 1.00 | 66.30 |
| | ATOM | 1230 | CD1 | PHE | 461 | 26.657 | 13.754 | 6.312 | 1.00 | 65.58 |
| | ATOM | 1231 | CD2 | PHE | 461 | 27.963 | 11.760 | 6.085 | 1.00 | 66.41 |
| | ATOM | 1232 | CE1 | PHE | 461 | 25.562 | 12.996 | 6.723 | 1.00 | 65.45 |
| | ATOM | 1233 | CE2 | PHE | 461 | 26.872 | 10.994 | 6.494 | 1.00 | 66.83 |
| 55 | ATOM | 1234 | CZ | PHE | 461 | 25.670 | 11.616 | 6.814 | 1.00 | 65.12 |
| | ATOM | 1235 | C | PHE | 461 | 31.463 | 13.604 | 5.004 | 1.00 | 68.38 |
| | ATOM | 1236 | O | PHE | 461 | 32.181 | 14.606 | 4.962 | 1.00 | 68.98 |
| | ATOM | 1237 | N | LEU | 462 | 31.542 | 12.601 | 4.132 | 1.00 | 69.57 |
| | ATOM | 1238 | CA | LEU | 462 | 32.511 | 12.545 | 3.039 | 1.00 | 71.68 |
| 60 | ATOM | 1239 | CB | LEU | 462 | 32.080 | 11.475 | 2.030 | 1.00 | 71.00 |
| | ATOM | 1240 | C | LEU | 462 | 32.810 | 13.856 | 2.304 | 1.00 | 72.40 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1241 | O | LEU | 462 | 33.725 | 14.590 | 2.680 | 1.00 | 73.45 |
| | ATOM | 1242 | N | SER | 463 | 32.043 | 14.141 | 1.253 | 1.00 | 73.22 |
| | ATOM | 1243 | CA | SER | 463 | 32.262 | 15.343 | 0.449 | 1.00 | 72.61 |
| | ATOM | 1244 | CB | SER | 463 | 32.544 | 14.942 | -1.005 | 1.00 | 73.38 |
| | ATOM | 1245 | C | SER | 463 | 31.126 | 16.362 | 0.491 | 1.00 | 71.17 |
| 10 | ATOM | 1246 | O | SER | 463 | 30.455 | 16.528 | 1.511 | 1.00 | 72.05 |
| | ATOM | 1247 | N | SER | 464 | 30.932 | 17.049 | -0.633 | 1.00 | 68.86 |
| | ATOM | 1248 | CA | SER | 464 | 29.892 | 18.063 | -0.759 | 1.00 | 66.06 |
| | ATOM | 1249 | CB | SER | 464 | 30.514 | 19.457 | -0.704 | 1.00 | 66.26 |
| | ATOM | 1250 | C | SER | 464 | 29.108 | 17.887 | -2.060 | 1.00 | 63.72 |
| 15 | ATOM | 1251 | O | SER | 464 | 28.657 | 18.862 | -2.662 | 1.00 | 62.88 |
| | ATOM | 1252 | N | THR | 465 | 28.954 | 16.638 | -2.493 | 1.00 | 60.93 |
| | ATOM | 1253 | CA | THR | 465 | 28.205 | 16.343 | -3.709 | 1.00 | 57.47 |
| | ATOM | 1254 | CB | THR | 465 | 28.185 | 14.824 | -4.004 | 1.00 | 57.80 |
| | ATOM | 1255 | OG1 | THR | 465 | 27.525 | 14.135 | -2.934 | 1.00 | 54.75 |
| 20 | ATOM | 1256 | CG2 | THR | 465 | 29.606 | 14.287 | -4.149 | 1.00 | 57.49 |
| | ATOM | 1257 | C | THR | 465 | 26.767 | 16.824 | -3.523 | 1.00 | 54.93 |
| | ATOM | 1258 | O | THR | 465 | 26.349 | 17.129 | -2.407 | 1.00 | 54.26 |
| | ATOM | 1259 | N | LEU | 466 | 26.013 | 16.892 | -4.614 | 1.00 | 51.85 |
| | ATOM | 1260 | CA | LEU | 466 | 24.625 | 17.330 | -4.550 | 1.00 | 49.25 |
| 25 | ATOM | 1261 | CB | LEU | 466 | 24.013 | 17.349 | -5.956 | 1.00 | 48.74 |
| | ATOM | 1262 | CG | LEU | 466 | 22.953 | 18.415 | -6.253 | 1.00 | 48.72 |
| | ATOM | 1263 | CD1 | LEU | 466 | 22.156 | 18.002 | -7.482 | 1.00 | 48.32 |
| | ATOM | 1264 | CD2 | LEU | 466 | 22.033 | 18.594 | -5.057 | 1.00 | 48.14 |
| | ATOM | 1265 | C | LEU | 466 | 23.817 | 16.397 | -3.650 | 1.00 | 48.16 |
| 30 | ATOM | 1266 | O | LEU | 466 | 22.961 | 16.845 | -2.883 | 1.00 | 45.90 |
| | ATOM | 1267 | N | LYS | 467 | 24.093 | 15.099 | -3.750 | 1.00 | 46.47 |
| | ATOM | 1268 | CA | LYS | 467 | 23.399 | 14.100 | -2.947 | 1.00 | 47.45 |
| | ATOM | 1269 | CB | LYS | 467 | 23.802 | 12.693 | -3.395 | 1.00 | 49.38 |
| | ATOM | 1270 | CG | LYS | 467 | 22.829 | 11.602 | -2.974 | 1.00 | 52.70 |
| 35 | ATOM | 1271 | CD | LYS | 467 | 23.561 | 10.301 | -2.682 | 1.00 | 56.48 |
| | ATOM | 1272 | CE | LYS | 467 | 23.105 | 9.180 | -3.604 | 1.00 | 59.54 |
| | ATOM | 1273 | NZ | LYS | 467 | 24.150 | 8.117 | -3.732 | 1.00 | 61.22 |
| | ATOM | 1274 | C | LYS | 467 | 23.738 | 14.284 | -1.472 | 1.00 | 46.89 |
| | ATOM | 1275 | O | LYS | 467 | 22.884 | 14.108 | -0.604 | 1.00 | 46.06 |
| 40 | ATOM | 1276 | N | SER | 468 | 24.989 | 14.644 | -1.202 | 1.00 | 45.82 |
| | ATOM | 1277 | CA | SER | 468 | 25.457 | 14.854 | 0.160 | 1.00 | 46.82 |
| | ATOM | 1278 | CB | SER | 468 | 26.976 | 15.050 | 0.173 | 1.00 | 47.85 |
| | ATOM | 1279 | OG | SER | 468 | 27.407 | 15.537 | 1.435 | 1.00 | 55.73 |
| | ATOM | 1280 | C | SER | 468 | 24.778 | 16.063 | 0.790 | 1.00 | 44.24 |
| 45 | ATOM | 1281 | O | SER | 468 | 24.473 | 16.062 | 1.983 | 1.00 | 42.98 |
| | ATOM | 1282 | N | LEU | 469 | 24.547 | 17.100 | -0.011 | 1.00 | 42.33 |
| | ATOM | 1283 | CA | LEU | 469 | 23.890 | 18.301 | 0.486 | 1.00 | 40.42 |
| | ATOM | 1284 | CB | LEU | 469 | 24.002 | 19.427 | -0.545 | 1.00 | 44.47 |
| | ATOM | 1285 | CG | LEU | 469 | 25.438 | 19.874 | -0.849 | 1.00 | 46.70 |
| 50 | ATOM | 1286 | CD1 | LEU | 469 | 25.514 | 20.477 | -2.246 | 1.00 | 46.70 |
| | ATOM | 1287 | CD2 | LEU | 469 | 25.890 | 20.883 | 0.199 | 1.00 | 47.32 |
| | ATOM | 1288 | C | LEU | 469 | 22.423 | 17.996 | 0.786 | 1.00 | 39.06 |
| | ATOM | 1289 | O | LEU | 469 | 21.856 | 18.505 | 1.760 | 1.00 | 34.97 |
| | ATOM | 1290 | N | GLU | 470 | 21.814 | 17.151 | -0.046 | 1.00 | 35.46 |
| 55 | ATOM | 1291 | CA | GLU | 470 | 20.418 | 16.768 | 0.145 | 1.00 | 34.38 |
| | ATOM | 1292 | CB | GLU | 470 | 19.914 | 15.963 | -1.052 | 1.00 | 38.02 |
| | ATOM | 1293 | CG | GLU | 470 | 19.772 | 16.773 | -2.329 | 1.00 | 42.67 |
| | ATOM | 1294 | CD | GLU | 470 | 19.339 | 15.923 | -3.509 | 1.00 | 48.30 |
| | ATOM | 1295 | OE1 | GLU | 470 | 19.671 | 14.716 | -3.538 | 1.00 | 50.53 |
| 60 | ATOM | 1296 | OE2 | GLU | 470 | 18.666 | 16.463 | -4.412 | 1.00 | 51.06 |
| | ATOM | 1297 | C | GLU | 470 | 20.290 | 15.916 | 1.403 | 1.00 | 34.37 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1298 | O | GLU | 470 | 19.321 | 16.035 | 2.157 | 1.00 | 32.60 |
| | ATOM | 1299 | N | GLU | 471 | 21.274 | 15.046 | 1.606 | 1.00 | 34.66 |
| | ATOM | 1300 | CA | GLU | 471 | 21.309 | 14.162 | 2.766 | 1.00 | 35.68 |
| | ATOM | 1301 | CB | GLU | 471 | 22.515 | 13.222 | 2.671 | 1.00 | 34.57 |
| | ATOM | 1302 | CG | GLU | 471 | 22.376 | 12.122 | 1.614 | 1.00 | 37.98 |
| 10 | ATOM | 1303 | CD | GLU | 471 | 21.476 | 10.989 | 2.063 | 1.00 | 39.79 |
| | ATOM | 1304 | OE1 | GLU | 471 | 20.268 | 11.027 | 1.743 | 1.00 | 41.12 |
| | ATOM | 1305 | OE2 | GLU | 471 | 21.974 | 10.061 | 2.737 | 1.00 | 32.11 |
| | ATOM | 1306 | C | GLU | 471 | 21.393 | 14.983 | 4.052 | 1.00 | 34.79 |
| | ATOM | 1307 | O | GLU | 471 | 20.596 | 14.793 | 4.969 | 1.00 | 32.80 |
| 15 | ATOM | 1308 | N | LYS | 472 | 22.358 | 15.898 | 4.112 | 1.00 | 33.93 |
| | ATOM | 1309 | CA | LYS | 472 | 22.518 | 16.739 | 5.291 | 1.00 | 35.58 |
| | ATOM | 1310 | CB | LYS | 472 | 23.683 | 17.710 | 5.097 | 1.00 | 39.11 |
| | ATOM | 1311 | CG | LYS | 472 | 25.050 | 17.050 | 5.138 | 1.00 | 41.47 |
| | ATOM | 1312 | CD | LYS | 472 | 26.080 | 17.957 | 5.794 | 1.00 | 46.97 |
| 20 | ATOM | 1313 | CE | LYS | 472 | 27.445 | 17.286 | 5.862 | 1.00 | 48.40 |
| | ATOM | 1314 | NZ | LYS | 472 | 27.850 | 16.702 | 4.547 | 1.00 | 51.55 |
| | ATOM | 1315 | C | LYS | 472 | 21.237 | 17.523 | 5.582 | 1.00 | 34.78 |
| | ATOM | 1316 | O | LYS | 472 | 20.795 | 17.607 | 6.724 | 1.00 | 33.95 |
| | ATOM | 1317 | N | ASP | 473 | 20.643 | 18.097 | 4.545 | 1.00 | 33.47 |
| 25 | ATOM | 1318 | CA | ASP | 473 | 19.420 | 18.865 | 4.720 | 1.00 | 34.63 |
| | ATOM | 1319 | CB | ASP | 473 | 18.923 | 19.404 | 3.380 | 1.00 | 37.21 |
| | ATOM | 1320 | CG | ASP | 473 | 17.654 | 20.221 | 3.522 | 1.00 | 43.24 |
| | ATOM | 1321 | OD1 | ASP | 473 | 16.559 | 19.687 | 3.230 | 1.00 | 45.20 |
| | ATOM | 1322 | OD2 | ASP | 473 | 17.750 | 21.396 | 3.932 | 1.00 | 45.59 |
| 30 | ATOM | 1323 | C | ASP | 473 | 18.339 | 17.998 | 5.338 | 1.00 | 32.93 |
| | ATOM | 1324 | O | ASP | 473 | 17.642 | 18.416 | 6.264 | 1.00 | 32.87 |
| | ATOM | 1325 | N | HIS | 474 | 18.199 | 16.784 | 4.827 | 1.00 | 32.74 |
| | ATOM | 1326 | CA | HIS | 474 | 17.185 | 15.882 | 5.343 | 1.00 | 32.21 |
| | ATOM | 1327 | CB | HIS | 474 | 17.185 | 14.575 | 4.568 | 1.00 | 32.79 |
| 35 | ATOM | 1328 | CG | HIS | 474 | 16.047 | 13.675 | 4.924 | 1.00 | 36.22 |
| | ATOM | 1329 | CD2 | HIS | 474 | 14.711 | 13.813 | 4.750 | 1.00 | 38.33 |
| | ATOM | 1330 | ND1 | HIS | 474 | 16.227 | 12.456 | 5.542 | 1.00 | 38.97 |
| | ATOM | 1331 | CE1 | HIS | 474 | 15.053 | 11.883 | 5.732 | 1.00 | 37.99 |
| | ATOM | 1332 | NE2 | HIS | 474 | 14.116 | 12.686 | 5.261 | 1.00 | 37.43 |
| 40 | ATOM | 1333 | C | HIS | 474 | 17.403 | 15.573 | 6.815 | 1.00 | 29.74 |
| | ATOM | 1334 | O | HIS | 474 | 16.460 | 15.543 | 7.596 | 1.00 | 29.90 |
| | ATOM | 1335 | N | ILE | 475 | 18.653 | 15.326 | 7.185 | 1.00 | 27.80 |
| | ATOM | 1336 | CA | ILE | 475 | 18.971 | 15.014 | 8.571 | 1.00 | 25.61 |
| | ATOM | 1337 | CB | ILE | 475 | 20.478 | 14.708 | 8.720 | 1.00 | 25.59 |
| 45 | ATOM | 1338 | CG2 | ILE | 475 | 20.877 | 14.713 | 10.193 | 1.00 | 27.17 |
| | ATOM | 1339 | CG1 | ILE | 475 | 20.787 | 13.341 | 8.092 | 1.00 | 26.17 |
| | ATOM | 1340 | CD1 | ILE | 475 | 22.258 | 13.071 | 7.849 | 1.00 | 27.07 |
| | ATOM | 1341 | C | ILE | 475 | 18.576 | 16.201 | 9.460 | 1.00 | 27.91 |
| | ATOM | 1342 | O | ILE | 475 | 17.928 | 16.038 | 10.485 | 1.00 | 29.16 |
| 50 | ATOM | 1343 | N | HIS | 476 | 18.956 | 17.404 | 9.054 | 1.00 | 29.41 |
| | ATOM | 1344 | CA | HIS | 476 | 18.621 | 18.575 | 9.846 | 1.00 | 29.73 |
| | ATOM | 1345 | CB | HIS | 476 | 19.342 | 19.796 | 9.281 | 1.00 | 32.27 |
| | ATOM | 1346 | CG | HIS | 476 | 20.777 | 19.867 | 9.699 | 1.00 | 39.44 |
| | ATOM | 1347 | CD2 | HIS | 476 | 21.355 | 19.707 | 10.915 | 1.00 | 39.81 |
| 55 | ATOM | 1348 | ND1 | HIS | 476 | 21.809 | 20.067 | 8.808 | 1.00 | 39.79 |
| | ATOM | 1349 | CE1 | HIS | 476 | 22.959 | 20.027 | 9.456 | 1.00 | 39.98 |
| | ATOM | 1350 | NE2 | HIS | 476 | 22.712 | 19.809 | 10.735 | 1.00 | 40.26 |
| | ATOM | 1351 | C | HIS | 476 | 17.120 | 18.810 | 9.948 | 1.00 | 31.40 |
| | ATOM | 1352 | O | HIS | 476 | 16.636 | 19.336 | 10.951 | 1.00 | 29.79 |
| 60 | ATOM | 1353 | N | ARG | 477 | 16.374 | 18.396 | 8.929 | 1.00 | 31.82 |
| | ATOM | 1354 | CA | ARG | 477 | 14.929 | 18.570 | 8.956 | 1.00 | 31.53 |

| | | | | | | | | | | |
|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1355 | CB | ARG | 477 | 14.343 | 18.376 | 7.557 | 1.00 | 34.95 |
| | ATOM | 1356 | CG | ARG | 477 | 14.425 | 19.627 | 6.700 | 1.00 | 40.46 |
| | ATOM | 1357 | CD | ARG | 477 | 13.698 | 19.445 | 5.370 | 1.00 | 45.22 |
| | ATOM | 1358 | NE | ARG | 477 | 14.107 | 20.456 | 4.399 | 1.00 | 53.05 |
| | ATOM | 1359 | CZ | ARG | 477 | 13.647 | 21.705 | 4.376 | 1.00 | 55.89 |
| 10 | ATOM | 1360 | NH1 | ARG | 477 | 12.756 | 22.106 | 5.274 | 1.00 | 56.17 |
| | ATOM | 1361 | NH2 | ARG | 477 | 14.084 | 22.558 | 3.457 | 1.00 | 59.49 |
| | ATOM | 1362 | C | ARG | 477 | 14.310 | 17.582 | 9.931 | 1.00 | 30.70 |
| | ATOM | 1363 | O | ARG | 477 | 13.360 | 17.903 | 10.649 | 1.00 | 30.24 |
| | ATOM | 1364 | N | VAL | 478 | 14.863 | 16.375 | 9.972 | 1.00 | 29.67 |
| 15 | ATOM | 1365 | CA | VAL | 478 | 14.351 | 15.369 | 10.887 | 1.00 | 29.68 |
| | ATOM | 1366 | CB | VAL | 478 | 14.937 | 13.975 | 10.575 | 1.00 | 32.01 |
| | ATOM | 1367 | CG1 | VAL | 478 | 14.461 | 12.973 | 11.609 | 1.00 | 32.93 |
| | ATOM | 1368 | CG2 | VAL | 478 | 14.506 | 13.528 | 9.169 | 1.00 | 31.00 |
| | ATOM | 1369 | C | VAL | 478 | 14.696 | 15.774 | 12.316 | 1.00 | 29.81 |
| 20 | ATOM | 1370 | O | VAL | 478 | 13.860 | 15.677 | 13.220 | 1.00 | 30.25 |
| | ATOM | 1371 | N | LEU | 479 | 15.929 | 16.232 | 12.516 | 1.00 | 28.81 |
| | ATOM | 1372 | CA | LEU | 479 | 16.360 | 16.674 | 13.836 | 1.00 | 28.74 |
| | ATOM | 1373 | CB | LEU | 479 | 17.799 | 17.210 | 13.779 | 1.00 | 26.65 |
| | ATOM | 1374 | CG | LEU | 479 | 18.910 | 16.152 | 13.853 | 1.00 | 26.05 |
| 25 | ATOM | 1375 | CD1 | LEU | 479 | 20.231 | 16.772 | 13.395 | 1.00 | 25.81 |
| | ATOM | 1376 | CD2 | LEU | 479 | 19.028 | 15.603 | 15.277 | 1.00 | 25.34 |
| | ATOM | 1377 | C | LEU | 479 | 15.411 | 17.777 | 14.313 | 1.00 | 29.54 |
| | ATOM | 1378 | O | LEU | 479 | 14.997 | 17.786 | 15.472 | 1.00 | 29.00 |
| | ATOM | 1379 | N | ASP | 480 | 15.076 | 18.703 | 13.415 | 1.00 | 31.52 |
| 30 | ATOM | 1380 | CA | ASP | 480 | 14.162 | 19.800 | 13.741 | 1.00 | 33.84 |
| | ATOM | 1381 | CB | ASP | 480 | 13.943 | 20.712 | 12.528 | 1.00 | 34.37 |
| | ATOM | 1382 | CG | ASP | 480 | 15.055 | 21.743 | 12.345 | 1.00 | 36.26 |
| | ATOM | 1383 | OD1 | ASP | 480 | 15.119 | 22.354 | 11.257 | 1.00 | 36.56 |
| | ATOM | 1384 | OD2 | ASP | 480 | 15.860 | 21.951 | 13.274 | 1.00 | 34.19 |
| 35 | ATOM | 1385 | C | ASP | 480 | 12.818 | 19.222 | 14.174 | 1.00 | 33.48 |
| | ATOM | 1386 | O | ASP | 480 | 12.186 | 19.724 | 15.105 | 1.00 | 33.89 |
| | ATOM | 1387 | N | LYS | 481 | 12.379 | 18.161 | 13.498 | 1.00 | 33.90 |
| | ATOM | 1388 | CA | LYS | 481 | 11.106 | 17.536 | 13.839 | 1.00 | 32.97 |
| | ATOM | 1389 | CB | LYS | 481 | 10.719 | 16.489 | 12.784 | 1.00 | 34.66 |
| 40 | ATOM | 1390 | C | LYS | 481 | 11.164 | 16.895 | 15.225 | 1.00 | 33.57 |
| | ATOM | 1391 | O | LYS | 481 | 10.167 | 16.869 | 15.943 | 1.00 | 35.37 |
| | ATOM | 1392 | N | ILE | 482 | 12.328 | 16.377 | 15.607 | 1.00 | 32.71 |
| | ATOM | 1393 | CA | ILE | 482 | 12.457 | 15.764 | 16.922 | 1.00 | 31.60 |
| | ATOM | 1394 | CB | ILE | 482 | 13.743 | 14.913 | 17.028 | 1.00 | 32.65 |
| 45 | ATOM | 1395 | CG2 | ILE | 482 | 13.877 | 14.338 | 18.430 | 1.00 | 32.50 |
| | ATOM | 1396 | CG1 | ILE | 482 | 13.697 | 13.785 | 15.995 | 1.00 | 32.72 |
| | ATOM | 1397 | CD1 | ILE | 482 | 14.978 | 12.969 | 15.908 | 1.00 | 33.37 |
| | ATOM | 1398 | C | ILE | 482 | 12.456 | 16.853 | 17.994 | 1.00 | 31.69 |
| | ATOM | 1399 | O | ILE | 482 | 11.946 | 16.649 | 19.097 | 1.00 | 29.98 |
| 50 | ATOM | 1400 | N | THR | 483 | 13.027 | 18.012 | 17.679 | 1.00 | 31.33 |
| | ATOM | 1401 | CA | THR | 483 | 13.022 | 19.109 | 18.644 | 1.00 | 31.71 |
| | ATOM | 1402 | CB | THR | 483 | 13.756 | 20.351 | 18.109 | 1.00 | 32.92 |
| | ATOM | 1403 | OG1 | THR | 483 | 15.111 | 20.012 | 17.788 | 1.00 | 29.99 |
| | ATOM | 1404 | CG2 | THR | 483 | 13.756 | 21.452 | 19.160 | 1.00 | 30.47 |
| 55 | ATOM | 1405 | C | THR | 483 | 11.559 | 19.483 | 18.920 | 1.00 | 32.85 |
| | ATOM | 1406 | O | THR | 483 | 11.146 | 19.598 | 20.070 | 1.00 | 31.83 |
| | ATOM | 1407 | N | ASP | 484 | 10.785 | 19.656 | 17.851 | 1.00 | 31.91 |
| | ATOM | 1408 | CA | ASP | 484 | 9.369 | 20.003 | 17.965 | 1.00 | 34.15 |
| | ATOM | 1409 | CB | ASP | 484 | 8.708 | 20.013 | 16.591 | 1.00 | 37.41 |
| 60 | ATOM | 1410 | CG | ASP | 484 | 9.270 | 21.080 | 15.680 | 1.00 | 42.02 |
| | ATOM | 1411 | OD1 | ASP | 484 | 9.871 | 22.045 | 16.198 | 1.00 | 43.26 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1412 | OD2 | ASP | 484 | 9.106 | 20.952 | 14.445 | 1.00 | 42.49 |
| | ATOM | 1413 | C | ASP | 484 | 8.657 | 18.985 | 18.840 | 1.00 | 33.16 |
| | ATOM | 1414 | O | ASP | 484 | 7.830 | 19.339 | 19.676 | 1.00 | 34.86 |
| | ATOM | 1415 | N | THR | 485 | 8.996 | 17.715 | 18.646 | 1.00 | 33.91 |
| | ATOM | 1416 | CA | THR | 485 | 8.396 | 16.635 | 19.414 | 1.00 | 34.41 |
| 10 | ATOM | 1417 | CB | THR | 485 | 8.875 | 15.268 | 18.885 | 1.00 | 33.58 |
| | ATOM | 1418 | OG1 | THR | 485 | 8.400 | 15.094 | 17.542 | 1.00 | 37.04 |
| | ATOM | 1419 | CG2 | THR | 485 | 8.347 | 14.138 | 19.751 | 1.00 | 30.89 |
| | ATOM | 1420 | C | THR | 485 | 8.708 | 16.757 | 20.903 | 1.00 | 35.15 |
| | ATOM | 1421 | O | THR | 485 | 7.818 | 16.600 | 21.744 | 1.00 | 31.99 |
| 15 | ATOM | 1422 | N | LEU | 486 | 9.966 | 17.046 | 21.229 | 1.00 | 33.77 |
| | ATOM | 1423 | CA | LEU | 486 | 10.368 | 17.192 | 22.621 | 1.00 | 34.31 |
| | ATOM | 1424 | CB | LEU | 486 | 11.879 | 17.448 | 22.721 | 1.00 | 32.00 |
| | ATOM | 1425 | CG | LEU | 486 | 12.776 | 16.201 | 22.754 | 1.00 | 34.99 |
| | ATOM | 1426 | CD1 | LEU | 486 | 14.233 | 16.613 | 22.521 | 1.00 | 32.65 |
| 20 | ATOM | 1427 | CD2 | LEU | 486 | 12.635 | 15.481 | 24.105 | 1.00 | 29.90 |
| | ATOM | 1428 | C | LEU | 486 | 9.597 | 18.348 | 23.256 | 1.00 | 34.87 |
| | ATOM | 1429 | O | LEU | 486 | 9.078 | 18.225 | 24.362 | 1.00 | 35.85 |
| | ATOM | 1430 | N | ILE | 487 | 9.513 | 19.469 | 22.548 | 1.00 | 35.59 |
| | ATOM | 1431 | CA | ILE | 487 | 8.787 | 20.625 | 23.064 | 1.00 | 36.79 |
| 25 | ATOM | 1432 | CB | ILE | 487 | 8.890 | 21.826 | 22.095 | 1.00 | 37.32 |
| | ATOM | 1433 | CG2 | ILE | 487 | 7.833 | 22.884 | 22.443 | 1.00 | 40.19 |
| | ATOM | 1434 | CG1 | ILE | 487 | 10.292 | 22.443 | 22.181 | 1.00 | 36.00 |
| | ATOM | 1435 | CD1 | ILE | 487 | 10.635 | 23.041 | 23.544 | 1.00 | 33.58 |
| | ATOM | 1436 | C | ILE | 487 | 7.315 | 20.257 | 23.276 | 1.00 | 38.56 |
| 30 | ATOM | 1437 | O | ILE | 487 | 6.708 | 20.628 | 24.282 | 1.00 | 38.52 |
| | ATOM | 1438 | N | HIS | 488 | 6.749 | 19.521 | 22.326 | 1.00 | 40.33 |
| | ATOM | 1439 | CA | HIS | 488 | 5.357 | 19.096 | 22.427 | 1.00 | 42.29 |
| | ATOM | 1440 | CB | HIS | 488 | 4.962 | 18.282 | 21.197 | 1.00 | 44.26 |
| | ATOM | 1441 | CG | HIS | 488 | 3.612 | 17.647 | 21.305 | 1.00 | 47.75 |
| 35 | ATOM | 1442 | CD2 | HIS | 488 | 2.369 | 18.175 | 21.214 | 1.00 | 47.46 |
| | ATOM | 1443 | ND1 | HIS | 488 | 3.440 | 16.298 | 21.534 | 1.00 | 51.09 |
| | ATOM | 1444 | CE1 | HIS | 488 | 2.148 | 16.023 | 21.577 | 1.00 | 51.15 |
| | ATOM | 1445 | NE2 | HIS | 488 | 1.477 | 17.144 | 21.385 | 1.00 | 50.22 |
| | ATOM | 1446 | C | HIS | 488 | 5.154 | 18.254 | 23.685 | 1.00 | 42.55 |
| 40 | ATOM | 1447 | O | HIS | 488 | 4.233 | 18.498 | 24.467 | 1.00 | 43.02 |
| | ATOM | 1448 | N | LEU | 489 | 6.022 | 17.266 | 23.879 | 1.00 | 39.91 |
| | ATOM | 1449 | CA | LEU | 489 | 5.936 | 16.399 | 25.048 | 1.00 | 39.93 |
| | ATOM | 1450 | CB | LEU | 489 | 7.087 | 15.396 | 25.048 | 1.00 | 38.83 |
| | ATOM | 1451 | CG | LEU | 489 | 6.961 | 14.242 | 24.056 | 1.00 | 39.31 |
| 45 | ATOM | 1452 | CD1 | LEU | 489 | 8.259 | 13.456 | 24.027 | 1.00 | 39.01 |
| | ATOM | 1453 | CD2 | LEU | 489 | 5.799 | 13.345 | 24.459 | 1.00 | 41.98 |
| | ATOM | 1454 | C | LEU | 489 | 5.973 | 17.203 | 26.339 | 1.00 | 40.24 |
| | ATOM | 1455 | O | LEU | 489 | 5.267 | 16.888 | 27.298 | 1.00 | 38.72 |
| | ATOM | 1456 | N | MET | 490 | 6.798 | 18.246 | 26.353 | 1.00 | 39.94 |
| 50 | ATOM | 1457 | CA | MET | 490 | 6.939 | 19.102 | 27.522 | 1.00 | 41.50 |
| | ATOM | 1458 | CB | MET | 490 | 8.208 | 19.953 | 27.394 | 1.00 | 39.15 |
| | ATOM | 1459 | CG | MET | 490 | 9.495 | 19.169 | 27.608 | 1.00 | 41.69 |
| | ATOM | 1460 | SD | MET | 490 | 10.978 | 20.106 | 27.161 | 1.00 | 35.76 |
| | ATOM | 1461 | CE | MET | 490 | 12.178 | 18.775 | 27.056 | 1.00 | 39.22 |
| 55 | ATOM | 1462 | C | MET | 490 | 5.718 | 20.004 | 27.717 | 1.00 | 42.33 |
| | ATOM | 1463 | O | MET | 490 | 5.296 | 20.258 | 28.848 | 1.00 | 41.09 |
| | ATOM | 1464 | N | ALA | 491 | 5.162 | 20.498 | 26.616 | 1.00 | 43.15 |
| | ATOM | 1465 | CA | ALA | 491 | 3.983 | 21.351 | 26.693 | 1.00 | 43.79 |
| | ATOM | 1466 | CB | ALA | 491 | 3.622 | 21.879 | 25.311 | 1.00 | 43.93 |
| 60 | ATOM | 1467 | C | ALA | 491 | 2.841 | 20.510 | 27.251 | 1.00 | 46.16 |
| | ATOM | 1468 | O | ALA | 491 | 2.073 | 20.967 | 28.095 | 1.00 | 44.69 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1469 | N | LYS | 492 | 2.752 | 19.268 | 26.783 | 1.00 | 46.29 |
| | ATOM | 1470 | CA | LYS | 492 | 1.711 | 18.351 | 27.222 | 1.00 | 49.90 |
| | ATOM | 1471 | CB | LYS | 492 | 1.772 | 17.053 | 26.411 | 1.00 | 50.03 |
| | ATOM | 1472 | CG | LYS | 492 | 1.087 | 17.135 | 25.062 | 1.00 | 53.81 |
| | ATOM | 1473 | CD | LYS | 492 | -0.002 | 16.084 | 24.930 | 1.00 | 59.00 |
| 10 | ATOM | 1474 | CE | LYS | 492 | -0.988 | 16.453 | 23.827 | 1.00 | 61.85 |
| | ATOM | 1475 | NZ | LYS | 492 | -1.351 | 15.281 | 22.976 | 1.00 | 62.89 |
| | ATOM | 1476 | C | LYS | 492 | 1.841 | 18.025 | 28.701 | 1.00 | 51.15 |
| | ATOM | 1477 | O | LYS | 492 | 0.845 | 17.784 | 29.379 | 1.00 | 53.37 |
| | ATOM | 1478 | N | ALA | 493 | 3.072 | 18.012 | 29.199 | 1.00 | 50.15 |
| 15 | ATOM | 1479 | CA | ALA | 493 | 3.321 | 17.706 | 30.600 | 1.00 | 49.17 |
| | ATOM | 1480 | CB | ALA | 493 | 4.777 | 17.314 | 30.794 | 1.00 | 50.39 |
| | ATOM | 1481 | C | ALA | 493 | 2.971 | 18.885 | 31.501 | 1.00 | 49.36 |
| | ATOM | 1482 | O | ALA | 493 | 3.089 | 18.799 | 32.723 | 1.00 | 51.57 |
| | ATOM | 1483 | N | GLY | 494 | 2.554 | 19.989 | 30.893 | 1.00 | 48.61 |
| 20 | ATOM | 1484 | CA | GLY | 494 | 2.185 | 21.159 | 31.671 | 1.00 | 46.92 |
| | ATOM | 1485 | C | GLY | 494 | 3.322 | 22.107 | 32.006 | 1.00 | 45.46 |
| | ATOM | 1486 | O | GLY | 494 | 3.206 | 22.921 | 32.919 | 1.00 | 43.58 |
| | ATOM | 1487 | N | LEU | 495 | 4.431 | 22.009 | 31.284 | 1.00 | 44.81 |
| | ATOM | 1488 | CA | LEU | 495 | 5.555 | 22.899 | 31.540 | 1.00 | 42.34 |
| 25 | ATOM | 1489 | CB | LEU | 495 | 6.847 | 22.293 | 30.988 | 1.00 | 43.79 |
| | ATOM | 1490 | CG | LEU | 495 | 7.712 | 21.459 | 31.936 | 1.00 | 40.99 |
| | ATOM | 1491 | CD1 | LEU | 495 | 7.022 | 20.156 | 32.260 | 1.00 | 44.70 |
| | ATOM | 1492 | CD2 | LEU | 495 | 9.072 | 21.189 | 31.270 | 1.00 | 42.12 |
| | ATOM | 1493 | C | LEU | 495 | 5.278 | 24.227 | 30.847 | 1.00 | 42.13 |
| 30 | ATOM | 1494 | O | LEU | 495 | 4.664 | 24.258 | 29.778 | 1.00 | 42.49 |
| | ATOM | 1495 | N | THR | 496 | 5.718 | 25.324 | 31.452 | 1.00 | 42.73 |
| | ATOM | 1496 | CA | THR | 496 | 5.521 | 26.636 | 30.845 | 1.00 | 43.56 |
| | ATOM | 1497 | CB | THR | 496 | 5.841 | 27.767 | 31.829 | 1.00 | 46.09 |
| | ATOM | 1498 | OG1 | THR | 496 | 7.222 | 27.688 | 32.208 | 1.00 | 43.92 |
| 35 | ATOM | 1499 | CG2 | THR | 496 | 4.965 | 27.662 | 33.064 | 1.00 | 45.63 |
| | ATOM | 1500 | C | THR | 496 | 6.471 | 26.764 | 29.660 | 1.00 | 45.54 |
| | ATOM | 1501 | O | THR | 496 | 7.370 | 25.939 | 29.488 | 1.00 | 43.39 |
| | ATOM | 1502 | N | LEU | 497 | 6.280 | 27.800 | 28.849 | 1.00 | 45.02 |
| | ATOM | 1503 | CA | LEU | 497 | 7.135 | 28.020 | 27.688 | 1.00 | 45.12 |
| 40 | ATOM | 1504 | CB | LEU | 497 | 6.710 | 29.286 | 26.944 | 1.00 | 46.62 |
| | ATOM | 1505 | CG | LEU | 497 | 5.933 | 29.080 | 25.640 | 1.00 | 50.20 |
| | ATOM | 1506 | CD1 | LEU | 497 | 5.886 | 30.397 | 24.875 | 1.00 | 50.95 |
| | ATOM | 1507 | CD2 | LEU | 497 | 6.589 | 27.990 | 24.798 | 1.00 | 50.91 |
| | ATOM | 1508 | C | LEU | 497 | 8.599 | 28.135 | 28.101 | 1.00 | 44.94 |
| 45 | ATOM | 1509 | O | LEU | 497 | 9.474 | 27.516 | 27.493 | 1.00 | 45.03 |
| | ATOM | 1510 | N | GLN | 498 | 8.862 | 28.927 | 29.137 | 1.00 | 41.14 |
| | ATOM | 1511 | CA | GLN | 498 | 10.221 | 29.101 | 29.627 | 1.00 | 40.54 |
| | ATOM | 1512 | CB | GLN | 498 | 10.246 | 30.140 | 30.743 | 1.00 | 43.82 |
| | ATOM | 1513 | CG | GLN | 498 | 11.585 | 30.270 | 31.437 | 1.00 | 43.37 |
| 50 | ATOM | 1514 | CD | GLN | 498 | 11.539 | 31.260 | 32.584 | 1.00 | 47.03 |
| | ATOM | 1515 | OE1 | GLN | 498 | 10.565 | 31.308 | 33.332 | 1.00 | 49.18 |
| | ATOM | 1516 | NE2 | GLN | 498 | 12.591 | 32.054 | 32.727 | 1.00 | 45.30 |
| | ATOM | 1517 | C | GLN | 498 | 10.777 | 27.773 | 30.145 | 1.00 | 39.39 |
| | ATOM | 1518 | O | GLN | 498 | 11.923 | 27.422 | 29.866 | 1.00 | 35.05 |
| 55 | ATOM | 1519 | N | GLN | 499 | 9.965 | 27.040 | 30.902 | 1.00 | 36.49 |
| | ATOM | 1520 | CA | GLN | 499 | 10.391 | 25.748 | 31.434 | 1.00 | 36.91 |
| | ATOM | 1521 | CB | GLN | 499 | 9.314 | 25.155 | 32.344 | 1.00 | 38.84 |
| | ATOM | 1522 | CG | GLN | 499 | 9.155 | 25.825 | 33.703 | 1.00 | 41.33 |
| | ATOM | 1523 | CD | GLN | 499 | 8.039 | 25.187 | 34.512 | 1.00 | 42.74 |
| 60 | ATOM | 1524 | OE1 | GLN | 499 | 7.027 | 24.760 | 33.955 | 1.00 | 45.44 |
| | ATOM | 1525 | NE2 | GLN | 499 | 8.222 | 25.107 | 35.829 | 1.00 | 43.48 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1526 | C | GLN | 499 | 10.655 | 24.773 | 30.285 | 1.00 | 35.03 |
| | ATOM | 1527 | O | GLN | 499 | 11.446 | 23.832 | 30.422 | 1.00 | 36.59 |
| | ATOM | 1528 | N | GLN | 500 | 9.980 | 24.994 | 29.162 | 1.00 | 34.14 |
| | ATOM | 1529 | CA | GLN | 500 | 10.136 | 24.138 | 27.990 | 1.00 | 34.65 |
| | ATOM | 1530 | CB | GLN | 500 | 9.042 | 24.436 | 26.958 | 1.00 | 33.90 |
| 10 | ATOM | 1531 | CG | GLN | 500 | 7.672 | 23.872 | 27.315 | 1.00 | 36.62 |
| | ATOM | 1532 | CD | GLN | 500 | 6.558 | 24.419 | 26.435 | 1.00 | 40.17 |
| | ATOM | 1533 | OE1 | GLN | 500 | 6.660 | 24.417 | 25.207 | 1.00 | 40.22 |
| | ATOM | 1534 | NE2 | GLN | 500 | 5.482 | 24.886 | 27.064 | 1.00 | 41.82 |
| | ATOM | 1535 | C | GLN | 500 | 11.511 | 24.350 | 27.358 | 1.00 | 34.96 |
| 15 | ATOM | 1536 | O | GLN | 500 | 12.256 | 23.387 | 27.124 | 1.00 | 30.79 |
| | ATOM | 1537 | N | HIS | 501 | 11.835 | 25.612 | 27.078 | 1.00 | 34.21 |
| | ATOM | 1538 | CA | HIS | 501 | 13.117 | 25.966 | 26.480 | 1.00 | 37.42 |
| | ATOM | 1539 | CB | HIS | 501 | 13.195 | 27.476 | 26.246 | 1.00 | 43.08 |
| | ATOM | 1540 | CG | HIS | 501 | 12.043 | 28.027 | 25.468 | 1.00 | 51.13 |
| 20 | ATOM | 1541 | CD2 | HIS | 501 | 11.534 | 27.678 | 24.263 | 1.00 | 53.05 |
| | ATOM | 1542 | ND1 | HIS | 501 | 11.264 | 29.068 | 25.926 | 1.00 | 54.54 |
| | ATOM | 1543 | CE1 | HIS | 501 | 10.325 | 29.337 | 25.037 | 1.00 | 54.36 |
| | ATOM | 1544 | NE2 | HIS | 501 | 10.466 | 28.508 | 24.018 | 1.00 | 55.19 |
| | ATOM | 1545 | C | HIS | 501 | 14.255 | 25.543 | 27.395 | 1.00 | 35.79 |
| 25 | ATOM | 1546 | O | HIS | 501 | 15.271 | 24.996 | 26.945 | 1.00 | 36.20 |
| | ATOM | 1547 | N | GLN | 502 | 14.086 | 25.799 | 28.685 | 1.00 | 33.90 |
| | ATOM | 1548 | CA | GLN | 502 | 15.110 | 25.438 | 29.650 | 1.00 | 32.18 |
| | ATOM | 1549 | CB | GLN | 502 | 14.740 | 25.977 | 31.033 | 1.00 | 35.84 |
| | ATOM | 1550 | CG | GLN | 502 | 14.787 | 27.498 | 31.113 | 1.00 | 32.66 |
| 30 | ATOM | 1551 | CD | GLN | 502 | 14.420 | 28.028 | 32.486 | 1.00 | 36.62 |
| | ATOM | 1552 | OE1 | GLN | 502 | 14.102 | 27.262 | 33.397 | 1.00 | 33.99 |
| | ATOM | 1553 | NE2 | GLN | 502 | 14.462 | 29.348 | 32.640 | 1.00 | 36.22 |
| | ATOM | 1554 | C | GLN | 502 | 15.340 | 23.932 | 29.716 | 1.00 | 31.79 |
| | ATOM | 1555 | O | GLN | 502 | 16.483 | 23.479 | 29.769 | 1.00 | 28.00 |
| 35 | ATOM | 1556 | N | ARG | 503 | 14.266 | 23.146 | 29.705 | 1.00 | 30.99 |
| | ATOM | 1557 | CA | ARG | 503 | 14.436 | 21.704 | 29.779 | 1.00 | 29.91 |
| | ATOM | 1558 | CB | ARG | 503 | 13.107 | 21.011 | 30.052 | 1.00 | 32.79 |
| | ATOM | 1559 | CG | ARG | 503 | 13.258 | 19.541 | 30.400 | 1.00 | 30.84 |
| | ATOM | 1560 | CD | ARG | 503 | 11.930 | 18.935 | 30.798 | 1.00 | 30.61 |
| 40 | ATOM | 1561 | NE | ARG | 503 | 12.021 | 17.490 | 30.992 | 1.00 | 28.50 |
| | ATOM | 1562 | CZ | ARG | 503 | 12.489 | 16.908 | 32.093 | 1.00 | 29.00 |
| | ATOM | 1563 | NH1 | ARG | 503 | 12.917 | 17.640 | 33.114 | 1.00 | 29.85 |
| | ATOM | 1564 | NH2 | ARG | 503 | 12.512 | 15.583 | 32.180 | 1.00 | 33.73 |
| | ATOM | 1565 | C | ARG | 503 | 15.051 | 21.152 | 28.496 | 1.00 | 29.89 |
| 45 | ATOM | 1566 | O | ARG | 503 | 15.895 | 20.259 | 28.548 | 1.00 | 29.69 |
| | ATOM | 1567 | N | LEU | 504 | 14.624 | 21.675 | 27.351 | 1.00 | 28.99 |
| | ATOM | 1568 | CA | LEU | 504 | 15.164 | 21.223 | 26.075 | 1.00 | 28.90 |
| | ATOM | 1569 | CB | LEU | 504 | 14.566 | 22.023 | 24.916 | 1.00 | 27.72 |
| | ATOM | 1570 | CG | LEU | 504 | 15.327 | 21.901 | 23.593 | 1.00 | 30.47 |
| 50 | ATOM | 1571 | CD1 | LEU | 504 | 15.252 | 20.453 | 23.117 | 1.00 | 31.74 |
| | ATOM | 1572 | CD2 | LEU | 504 | 14.742 | 22.843 | 22.542 | 1.00 | 29.85 |
| | ATOM | 1573 | C | LEU | 504 | 16.681 | 21.419 | 26.089 | 1.00 | 29.69 |
| | ATOM | 1574 | O | LEU | 504 | 17.439 | 20.536 | 25.672 | 1.00 | 26.38 |
| | ATOM | 1575 | N | ALA | 505 | 17.114 | 22.585 | 26.564 | 1.00 | 28.51 |
| 55 | ATOM | 1576 | CA | ALA | 505 | 18.535 | 22.899 | 26.632 | 1.00 | 25.98 |
| | ATOM | 1577 | CB | ALA | 505 | 18.735 | 24.361 | 27.039 | 1.00 | 29.86 |
| | ATOM | 1578 | C | ALA | 505 | 19.261 | 21.977 | 27.604 | 1.00 | 26.67 |
| | ATOM | 1579 | O | ALA | 505 | 20.340 | 21.462 | 27.290 | 1.00 | 25.54 |
| | ATOM | 1580 | N | GLN | 506 | 18.677 | 21.771 | 28.784 | 1.00 | 23.59 |
| 60 | ATOM | 1581 | CA | GLN | 506 | 19.299 | 20.907 | 29.785 | 1.00 | 27.67 |
| | ATOM | 1582 | CB | GLN | 506 | 18.434 | 20.796 | 31.043 | 1.00 | 27.75 |

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|----|------|------|-----|------|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1583 | CG | GLN | 506 | 18.414 | 22.027 | 31.945 | 1.00 | 32.48 |
| | ATOM | 1584 | CD | GLN | 506 | 17.111 | 22.116 | 32.736 | 1.00 | 38.40 |
| | ATOM | 1585 | OE1 | GLN | 506 | 16.319 | 21.167 | 32.754 | 1.00 | 35.97 |
| | ATOM | 1586 | NE2 | GLN | 506 | 16.879 | 23.257 | 33.386 | 1.00 | 38.07 |
| | ATOM | 1587 | C | GLN | 506 | 19.500 | 19.509 | 29.217 | 1.00 | 24.53 |
| 10 | ATOM | 1588 | O | GLN | 506 | 20.536 | 18.889 | 29.441 | 1.00 | 26.42 |
| | ATOM | 1589 | N | LEU | 507 | 18.505 | 19.017 | 28.484 | 1.00 | 26.78 |
| | ATOM | 1590 | CA | LEU | 507 | 18.578 | 17.678 | 27.902 | 1.00 | 26.18 |
| | ATOM | 1591 | CB | LEU | 507 | 17.225 | 17.286 | 27.295 | 1.00 | 31.48 |
| | ATOM | 1592 | CG | LEU | 507 | 16.052 | 16.961 | 28.231 | 1.00 | 32.59 |
| 15 | ATOM | 1593 | CD1 | LEU | 507 | 14.836 | 16.561 | 27.389 | 1.00 | 33.78 |
| | ATOM | 1594 | CD2 | LEU | 507 | 16.431 | 15.838 | 29.174 | 1.00 | 30.18 |
| | ATOM | 1595 | C | LEU | 507 | 19.652 | 17.583 | 26.819 | 1.00 | 26.03 |
| | ATOM | 1596 | O | LEU | 507 | 20.421 | 16.621 | 26.771 | 1.00 | 27.28 |
| | ATOM | 1597 | N | LEU | 508 | 19.713 | 18.583 | 25.950 | 1.00 | 24.31 |
| 20 | ATOM | 1598 | CA | LEU | 508 | 20.690 | 18.557 | 24.863 | 1.00 | 23.68 |
| | ATOM | 1599 | CB | LEU | 508 | 20.339 | 19.629 | 23.828 | 1.00 | 23.91 |
| | ATOM | 1600 | CG | LEU | 508 | 19.004 | 19.436 | 23.102 | 1.00 | 24.68 |
| | ATOM | 1601 | CD1 | LEU | 508 | 18.905 | 20.416 | 21.945 | 1.00 | 25.11 |
| | ATOM | 1602 | CD2 | LEU | 508 | 18.903 | 17.994 | 22.580 | 1.00 | 27.53 |
| 25 | ATOM | 1603 | C | LEU | 508 | 22.127 | 18.727 | 25.341 | 1.00 | 22.93 |
| | ATOM | 1604 | O | LEU | 508 | 23.062 | 18.200 | 24.736 | 1.00 | 21.36 |
| | ATOM | 1605 | N | LEU | 509 | 22.302 | 19.451 | 26.441 | 1.00 | 23.86 |
| | ATOM | 1606 | CA | LEU | 509 | 23.637 | 19.661 | 26.991 | 1.00 | 26.28 |
| | ATOM | 1607 | CB | LEU | 509 | 23.598 | 20.735 | 28.095 | 1.00 | 28.08 |
| 30 | ATOM | 1608 | CG | LEU | 509 | 23.578 | 22.214 | 27.672 | 1.00 | 33.98 |
| | ATOM | 1609 | CD1 | LEU | 509 | 23.529 | 23.114 | 28.921 | 1.00 | 35.23 |
| | ATOM | 1610 | CD2 | LEU | 509 | 24.818 | 22.525 | 26.856 | 1.00 | 30.48 |
| | ATOM | 1611 | C | LEU | 509 | 24.154 | 18.327 | 27.540 | 1.00 | 26.08 |
| | ATOM | 1612 | O | LEU | 509 | 25.354 | 18.068 | 27.547 | 1.00 | 23.92 |
| 35 | ATOM | 1613 | N | ILE | 510 | 23.254 | 17.462 | 27.993 | 1.00 | 24.60 |
| | ATOM | 1614 | CA | ILE | 510 | 23.712 | 16.172 | 28.496 | 1.00 | 25.12 |
| | ATOM | 1615 | CB | ILE | 510 | 22.568 | 15.368 | 29.161 | 1.00 | 28.51 |
| | ATOM | 1616 | CG2 | ILE | 510 | 23.051 | 13.965 | 29.506 | 1.00 | 31.67 |
| | ATOM | 1617 | CG1 | ILE | 510 | 22.141 | 16.060 | 30.459 | 1.00 | 31.18 |
| 40 | ATOM | 1618 | CD1 | ILE | 510 | 20.712 | 15.749 | 30.882 | 1.00 | 37.16 |
| | ATOM | 1619 | C | ILE | 510 | 24.337 | 15.351 | 27.364 | 1.00 | 23.86 |
| | ATOM | 1620 | O | ILE | 510 | 25.225 | 14.534 | 27.600 | 1.00 | 24.14 |
| | ATOM | 1621 | N | LEU | 511 | 23.889 | 15.586 | 26.133 | 1.00 | 25.10 |
| | ATOM | 1622 | CA | LEU | 511 | 24.420 | 14.862 | 24.977 | 1.00 | 25.63 |
| 45 | ATOM | 1623 | CB | LEU | 511 | 23.628 | 15.225 | 23.714 | 1.00 | 23.89 |
| | ATOM | 1624 | CG | LEU | 511 | 22.152 | 14.801 | 23.659 | 1.00 | 25.78 |
| | ATOM | 1625 | CD1 | LEU | 511 | 21.648 | 14.920 | 22.224 | 1.00 | 26.55 |
| | ATOM | 1626 | CD2 | LEU | 511 | 21.990 | 13.363 | 24.146 | 1.00 | 26.29 |
| | ATOM | 1627 | C | LEU | 511 | 25.912 | 15.152 | 24.771 | 1.00 | 27.10 |
| 50 | ATOM | 1628 | O | LEU | 511 | 26.641 | 14.332 | 24.214 | 1.00 | 24.98 |
| | ATOM | 1629 | N | SER | 512 | 26.372 | 16.319 | 25.213 | 1.00 | 24.75 |
| | ATOM | 1630 | CA | SER | 512 | 27.787 | 16.637 | 25.076 | 1.00 | 23.68 |
| | ATOM | 1631 | CB | SER | 512 | 28.023 | 18.129 | 25.358 | 1.00 | 26.12 |
| | ATOM | 1632 | OG | SER | 512 | 29.271 | 18.327 | 25.986 | 1.00 | 37.17 |
| 55 | ATOM | 1633 | C | SER | 512 | 28.594 | 15.765 | 26.050 | 1.00 | 23.15 |
| | ATOM | 1634 | O | SER | 512 | 29.742 | 15.383 | 25.769 | 1.00 | 22.15 |
| | ATOM | 1635 | N | AHIS | 513 | 27.993 | 15.456 | 27.192 | 0.50 | 21.53 |
| | ATOM | 1636 | N | BHIS | 513 | 28.008 | 15.453 | 27.202 | 0.50 | 20.99 |
| | ATOM | 1637 | CA | AHIS | 513 | 28.645 | 14.624 | 28.196 | 0.50 | 21.79 |
| 60 | ATOM | 1638 | CA | BHIS | 513 | 28.696 | 14.607 | 28.174 | 0.50 | 20.94 |
| | ATOM | 1639 | CB | AHIS | 513 | 27.920 | 14.776 | 29.536 | 0.50 | 23.59 |

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|----|------|------|-----|------|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1640 | CB | BHIS | 513 | 27.991 | 14.636 | 29.536 | 0.50 | 21.59 |
| | ATOM | 1641 | CG | AHIS | 513 | 28.145 | 16.109 | 30.179 | 0.50 | 27.34 |
| | ATOM | 1642 | CG | BHIS | 513 | 28.800 | 14.032 | 30.642 | 0.50 | 23.94 |
| | ATOM | 1643 | CD2 | AHIS | 513 | 29.223 | 16.616 | 30.824 | 0.50 | 27.56 |
| | ATOM | 1644 | CD2 | BHIS | 513 | 30.095 | 14.211 | 31.001 | 0.50 | 24.22 |
| 10 | ATOM | 1645 | ND1 | AHIS | 513 | 27.204 | 17.117 | 30.160 | 0.50 | 30.62 |
| | ATOM | 1646 | ND1 | BHIS | 513 | 28.285 | 13.105 | 31.523 | 0.50 | 27.00 |
| | ATOM | 1647 | CE1 | AHIS | 513 | 27.693 | 18.185 | 30.763 | 0.50 | 26.32 |
| | ATOM | 1648 | CE1 | BHIS | 513 | 29.225 | 12.740 | 32.376 | 0.50 | 24.40 |
| | ATOM | 1649 | NE2 | AHIS | 513 | 28.916 | 17.908 | 31.176 | 0.50 | 28.30 |
| 15 | ATOM | 1650 | NE2 | BHIS | 513 | 30.334 | 13.396 | 32.081 | 0.50 | 25.54 |
| | ATOM | 1651 | C | AHIS | 513 | 28.666 | 13.164 | 27.738 | 0.50 | 19.81 |
| | ATOM | 1652 | C | BHIS | 513 | 28.720 | 13.171 | 27.652 | 0.50 | 19.42 |
| | ATOM | 1653 | O | AHIS | 513 | 29.601 | 12.426 | 28.026 | 0.50 | 22.45 |
| | ATOM | 1654 | O | BHIS | 513 | 29.707 | 12.457 | 27.809 | 0.50 | 22.62 |
| 20 | ATOM | 1655 | N | ILE | 514 | 27.633 | 12.753 | 27.015 | 1.00 | 20.76 |
| | ATOM | 1656 | CA | ILE | 514 | 27.572 | 11.396 | 26.492 | 1.00 | 20.94 |
| | ATOM | 1657 | CB | ILE | 514 | 26.154 | 11.086 | 25.953 | 1.00 | 27.76 |
| | ATOM | 1658 | CG2 | ILE | 514 | 26.169 | 9.800 | 25.123 | 1.00 | 28.26 |
| | ATOM | 1659 | CG1 | ILE | 514 | 25.185 | 10.965 | 27.139 | 1.00 | 27.91 |
| 25 | ATOM | 1660 | CD1 | ILE | 514 | 23.752 | 10.649 | 26.753 | 1.00 | 34.31 |
| | ATOM | 1661 | C | ILE | 514 | 28.641 | 11.256 | 25.398 | 1.00 | 20.66 |
| | ATOM | 1662 | O | ILE | 514 | 29.298 | 10.226 | 25.285 | 1.00 | 22.21 |
| | ATOM | 1663 | N | ARG | 515 | 28.825 | 12.294 | 24.589 | 1.00 | 20.48 |
| | ATOM | 1664 | CA | ARG | 515 | 29.861 | 12.243 | 23.554 | 1.00 | 21.98 |
| 30 | ATOM | 1665 | CB | ARG | 515 | 29.861 | 13.535 | 22.726 | 1.00 | 23.11 |
| | ATOM | 1666 | CG | ARG | 515 | 31.003 | 13.611 | 21.737 | 1.00 | 25.76 |
| | ATOM | 1667 | CD | ARG | 515 | 30.664 | 12.818 | 20.491 | 1.00 | 28.55 |
| | ATOM | 1668 | NE | ARG | 515 | 29.580 | 13.482 | 19.788 | 1.00 | 36.24 |
| | ATOM | 1669 | CZ | ARG | 515 | 29.615 | 13.827 | 18.508 | 1.00 | 38.91 |
| 35 | ATOM | 1670 | NH1 | ARG | 515 | 30.689 | 13.566 | 17.776 | 1.00 | 35.37 |
| | ATOM | 1671 | NH2 | ARG | 515 | 28.579 | 14.459 | 17.971 | 1.00 | 40.27 |
| | ATOM | 1672 | C | ARG | 515 | 31.221 | 12.087 | 24.225 | 1.00 | 21.29 |
| | ATOM | 1673 | O | ARG | 515 | 32.068 | 11.305 | 23.795 | 1.00 | 20.06 |
| | ATOM | 1674 | N | HIS | 516 | 31.420 | 12.844 | 25.293 | 1.00 | 23.23 |
| 40 | ATOM | 1675 | CA | HIS | 516 | 32.675 | 12.812 | 26.034 | 1.00 | 24.75 |
| | ATOM | 1676 | CB | HIS | 516 | 32.566 | 13.794 | 27.206 | 1.00 | 24.03 |
| | ATOM | 1677 | CG | HIS | 516 | 33.826 | 13.948 | 27.990 | 1.00 | 31.42 |
| | ATOM | 1678 | CD2 | HIS | 516 | 34.138 | 13.587 | 29.257 | 1.00 | 35.87 |
| | ATOM | 1679 | ND1 | HIS | 516 | 34.938 | 14.586 | 27.489 | 1.00 | 33.59 |
| 45 | ATOM | 1680 | CE1 | HIS | 516 | 35.882 | 14.613 | 28.411 | 1.00 | 35.70 |
| | ATOM | 1681 | NE2 | HIS | 516 | 35.422 | 14.013 | 29.495 | 1.00 | 33.35 |
| | ATOM | 1682 | C | HIS | 516 | 32.965 | 11.390 | 26.537 | 1.00 | 24.02 |
| | ATOM | 1683 | O | HIS | 516 | 34.059 | 10.852 | 26.362 | 1.00 | 23.66 |
| | ATOM | 1684 | N | MET | 517 | 31.969 | 10.786 | 27.168 | 1.00 | 20.91 |
| 50 | ATOM | 1685 | CA | MET | 517 | 32.109 | 9.436 | 27.684 | 1.00 | 24.21 |
| | ATOM | 1686 | CB | MET | 517 | 30.837 | 9.038 | 28.424 | 1.00 | 23.88 |
| | ATOM | 1687 | CG | MET | 517 | 30.607 | 9.903 | 29.652 | 1.00 | 26.32 |
| | ATOM | 1688 | SD | MET | 517 | 29.435 | 9.222 | 30.790 | 1.00 | 26.67 |
| | ATOM | 1689 | CE | MET | 517 | 27.914 | 9.390 | 29.807 | 1.00 | 23.26 |
| 55 | ATOM | 1690 | C | MET | 517 | 32.399 | 8.448 | 26.564 | 1.00 | 23.26 |
| | ATOM | 1691 | O | MET | 517 | 33.213 | 7.547 | 26.728 | 1.00 | 26.08 |
| | ATOM | 1692 | N | SER | 518 | 31.736 | 8.612 | 25.423 | 1.00 | 21.93 |
| | ATOM | 1693 | CA | SER | 518 | 31.977 | 7.717 | 24.301 | 1.00 | 23.08 |
| | ATOM | 1694 | CB | SER | 518 | 30.976 | 8.027 | 23.173 | 1.00 | 22.02 |
| 60 | ATOM | 1695 | OG | SER | 518 | 31.283 | 7.336 | 21.978 | 1.00 | 24.01 |
| | ATOM | 1696 | C | SER | 518 | 33.432 | 7.862 | 23.810 | 1.00 | 25.15 |

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|----|------|------|-----|------|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1697 | O | SER | 518 | 34.111 | 6.866 | 23.532 | 1.00 | 22.94 |
| | ATOM | 1698 | N | ASN | 519 | 33.923 | 9.097 | 23.713 | 1.00 | 22.42 |
| | ATOM | 1699 | CA | ASN | 519 | 35.295 | 9.309 | 23.260 | 1.00 | 21.87 |
| | ATOM | 1700 | CB | ASN | 519 | 35.605 | 10.807 | 23.157 | 1.00 | 24.46 |
| | ATOM | 1701 | CG | ASN | 519 | 34.864 | 11.469 | 22.021 | 1.00 | 29.02 |
| 10 | ATOM | 1702 | OD1 | ASN | 519 | 34.661 | 10.864 | 20.965 | 1.00 | 31.93 |
| | ATOM | 1703 | ND2 | ASN | 519 | 34.459 | 12.715 | 22.224 | 1.00 | 28.81 |
| | ATOM | 1704 | C | ASN | 519 | 36.292 | 8.643 | 24.201 | 1.00 | 21.46 |
| | ATOM | 1705 | O | ASN | 519 | 37.251 | 8.015 | 23.752 | 1.00 | 23.56 |
| | ATOM | 1706 | N | LYS | 520 | 36.070 | 8.782 | 25.504 | 1.00 | 23.23 |
| 15 | ATOM | 1707 | CA | LYS | 520 | 36.964 | 8.171 | 26.488 | 1.00 | 26.35 |
| | ATOM | 1708 | CB | LYS | 520 | 36.581 | 8.592 | 27.912 | 1.00 | 27.53 |
| | ATOM | 1709 | CG | LYS | 520 | 36.618 | 10.101 | 28.174 | 1.00 | 33.74 |
| | ATOM | 1710 | CD | LYS | 520 | 37.962 | 10.710 | 27.811 | 1.00 | 42.09 |
| | ATOM | 1711 | CE | LYS | 520 | 39.047 | 10.307 | 28.802 | 1.00 | 43.97 |
| 20 | ATOM | 1712 | NZ | LYS | 520 | 39.858 | 11.480 | 29.254 | 1.00 | 48.07 |
| | ATOM | 1713 | C | LYS | 520 | 36.899 | 6.644 | 26.376 | 1.00 | 27.71 |
| | ATOM | 1714 | O | LYS | 520 | 37.913 | 5.957 | 26.501 | 1.00 | 27.15 |
| | ATOM | 1715 | N | GLY | 521 | 35.704 | 6.117 | 26.141 | 1.00 | 25.02 |
| | ATOM | 1716 | CA | GLY | 521 | 35.562 | 4.676 | 26.003 | 1.00 | 26.67 |
| 25 | ATOM | 1717 | C | GLY | 521 | 36.254 | 4.168 | 24.753 | 1.00 | 27.06 |
| | ATOM | 1718 | O | GLY | 521 | 36.924 | 3.128 | 24.775 | 1.00 | 26.84 |
| | ATOM | 1719 | N | AMET | 522 | 36.101 | 4.893 | 23.650 | 0.50 | 25.87 |
| | ATOM | 1720 | N | BMET | 522 | 36.095 | 4.908 | 23.658 | 0.50 | 27.62 |
| | ATOM | 1721 | CA | AMET | 522 | 36.727 | 4.491 | 22.401 | 0.50 | 27.27 |
| 30 | ATOM | 1722 | CA | BMET | 522 | 36.703 | 4.551 | 22.384 | 0.50 | 30.14 |
| | ATOM | 1723 | CB | AMET | 522 | 36.267 | 5.396 | 21.260 | 0.50 | 26.50 |
| | ATOM | 1724 | CB | BMET | 522 | 36.252 | 5.525 | 21.288 | 0.50 | 32.46 |
| | ATOM | 1725 | CG | AMET | 522 | 34.827 | 5.162 | 20.866 | 0.50 | 25.05 |
| | ATOM | 1726 | CG | BMET | 522 | 35.681 | 4.854 | 20.045 | 0.50 | 35.70 |
| 35 | ATOM | 1727 | SD | AMET | 522 | 34.585 | 3.587 | 20.020 | 0.50 | 27.07 |
| | ATOM | 1728 | SD | BMET | 522 | 34.197 | 5.672 | 19.408 | 0.50 | 40.01 |
| | ATOM | 1729 | CE | AMET | 522 | 33.142 | 4.017 | 19.031 | 0.50 | 31.29 |
| | ATOM | 1730 | CE | BMET | 522 | 34.733 | 6.085 | 17.745 | 0.50 | 42.12 |
| | ATOM | 1731 | C | AMET | 522 | 38.242 | 4.532 | 22.512 | 0.50 | 28.99 |
| 40 | ATOM | 1732 | C | BMET | 522 | 38.224 | 4.567 | 22.483 | 0.50 | 30.76 |
| | ATOM | 1733 | O | AMET | 522 | 38.939 | 3.743 | 21.870 | 0.50 | 31.65 |
| | ATOM | 1734 | O | BMET | 522 | 38.905 | 3.793 | 21.807 | 0.50 | 32.87 |
| | ATOM | 1735 | N | GLU | 523 | 38.749 | 5.452 | 23.324 | 1.00 | 30.85 |
| | ATOM | 1736 | CA | GLU | 523 | 40.190 | 5.576 | 23.513 | 1.00 | 34.09 |
| 45 | ATOM | 1737 | CB | GLU | 523 | 40.515 | 6.725 | 24.480 | 1.00 | 35.59 |
| | ATOM | 1738 | CG | GLU | 523 | 40.658 | 8.079 | 23.784 | 1.00 | 43.35 |
| | ATOM | 1739 | CD | GLU | 523 | 40.560 | 9.265 | 24.739 | 1.00 | 46.63 |
| | ATOM | 1740 | OE1 | GLU | 523 | 39.832 | 10.240 | 24.416 | 1.00 | 47.64 |
| | ATOM | 1741 | OE2 | GLU | 523 | 41.212 | 9.225 | 25.805 | 1.00 | 43.09 |
| 50 | ATOM | 1742 | C | GLU | 523 | 40.718 | 4.260 | 24.061 | 1.00 | 34.62 |
| | ATOM | 1743 | O | GLU | 523 | 41.733 | 3.747 | 23.596 | 1.00 | 33.87 |
| | ATOM | 1744 | N | HIS | 524 | 40.021 | 3.700 | 25.042 | 1.00 | 36.33 |
| | ATOM | 1745 | CA | HIS | 524 | 40.455 | 2.427 | 25.607 | 1.00 | 39.20 |
| | ATOM | 1746 | CB | HIS | 524 | 39.678 | 2.093 | 26.878 | 1.00 | 40.75 |
| 55 | ATOM | 1747 | CG | HIS | 524 | 40.061 | 0.774 | 27.473 | 1.00 | 48.10 |
| | ATOM | 1748 | CD2 | HIS | 524 | 41.192 | 0.376 | 28.104 | 1.00 | 48.56 |
| | ATOM | 1749 | ND1 | HIS | 524 | 39.247 | -0.338 | 27.412 | 1.00 | 48.84 |
| | ATOM | 1750 | CE1 | HIS | 524 | 39.859 | -1.362 | 27.978 | 1.00 | 50.19 |
| | ATOM | 1751 | NE2 | HIS | 524 | 41.041 | -0.956 | 28.407 | 1.00 | 51.61 |
| 60 | ATOM | 1752 | C | HIS | 524 | 40.290 | 1.282 | 24.613 | 1.00 | 38.06 |
| | ATOM | 1753 | O | HIS | 524 | 41.226 | 0.521 | 24.371 | 1.00 | 38.18 |

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|----|------|------|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 1754 | N | LEU | 525 | 39.101 | 1.162 | 24.034 | 1.00 | 36.96 |
| | ATOM | 1755 | CA | LEU | 525 | 38.831 | 0.093 | 23.084 | 1.00 | 37.40 |
| | ATOM | 1756 | CB | LEU | 525 | 37.416 | 0.241 | 22.514 | 1.00 | 35.89 |
| | ATOM | 1757 | CG | LEU | 525 | 36.268 | 0.107 | 23.527 | 1.00 | 33.17 |
| | ATOM | 1758 | CD1 | LEU | 525 | 34.936 | 0.246 | 22.811 | 1.00 | 31.77 |
| 10 | ATOM | 1759 | CD2 | LEU | 525 | 36.343 | -1.240 | 24.238 | 1.00 | 35.92 |
| | ATOM | 1760 | C | LEU | 525 | 39.859 | 0.057 | 21.954 | 1.00 | 41.32 |
| | ATOM | 1761 | O | LEU | 525 | 40.244 | -1.015 | 21.487 | 1.00 | 40.76 |
| | ATOM | 1762 | N | TYR | 526 | 40.314 | 1.227 | 21.522 | 1.00 | 43.68 |
| | ATOM | 1763 | CA | TYR | 526 | 41.300 | 1.297 | 20.449 | 1.00 | 49.00 |
| 15 | ATOM | 1764 | CB | TYR | 526 | 41.376 | 2.722 | 19.890 | 1.00 | 51.86 |
| | ATOM | 1765 | CG | TYR | 526 | 42.305 | 2.878 | 18.704 | 1.00 | 57.70 |
| | ATOM | 1766 | CD1 | TYR | 526 | 41.835 | 2.718 | 17.400 | 1.00 | 58.93 |
| | ATOM | 1767 | CE1 | TYR | 526 | 42.681 | 2.875 | 16.305 | 1.00 | 61.21 |
| | ATOM | 1768 | CD2 | TYR | 526 | 43.653 | 3.200 | 18.883 | 1.00 | 58.58 |
| 20 | ATOM | 1769 | CE2 | TYR | 526 | 44.510 | 3.359 | 17.790 | 1.00 | 61.15 |
| | ATOM | 1770 | CZ | TYR | 526 | 44.016 | 3.194 | 16.505 | 1.00 | 61.09 |
| | ATOM | 1771 | OH | TYR | 526 | 44.851 | 3.343 | 15.417 | 1.00 | 63.79 |
| | ATOM | 1772 | C | TYR | 526 | 42.671 | 0.871 | 20.964 | 1.00 | 50.14 |
| | ATOM | 1773 | O | TYR | 526 | 43.471 | 0.303 | 20.223 | 1.00 | 50.73 |
| 25 | ATOM | 1774 | N | SER | 527 | 42.930 | 1.139 | 22.240 | 1.00 | 52.72 |
| | ATOM | 1775 | CA | SER | 527 | 44.205 | 0.790 | 22.857 | 1.00 | 55.88 |
| | ATOM | 1776 | CB | SER | 527 | 44.351 | 1.516 | 24.199 | 1.00 | 55.00 |
| | ATOM | 1777 | OG | SER | 527 | 43.752 | 0.788 | 25.257 | 1.00 | 52.46 |
| | ATOM | 1778 | C | SER | 527 | 44.365 | -0.718 | 23.054 | 1.00 | 60.39 |
| 30 | ATOM | 1779 | O | SER | 527 | 45.398 | -1.185 | 23.534 | 1.00 | 60.43 |
| | ATOM | 1780 | N | MET | 528 | 43.335 | -1.472 | 22.678 | 1.00 | 63.86 |
| | ATOM | 1781 | CA | MET | 528 | 43.347 | -2.929 | 22.788 | 1.00 | 67.95 |
| | ATOM | 1782 | CB | MET | 528 | 42.534 | -3.381 | 24.008 | 1.00 | 67.85 |
| | ATOM | 1783 | CG | MET | 528 | 41.237 | -2.606 | 24.222 | 1.00 | 70.10 |
| 35 | ATOM | 1784 | SD | MET | 528 | 39.895 | -3.569 | 24.983 | 1.00 | 71.70 |
| | ATOM | 1785 | CE | MET | 528 | 39.231 | -4.412 | 23.554 | 1.00 | 72.57 |
| | ATOM | 1786 | C | MET | 528 | 42.726 | -3.502 | 21.513 | 1.00 | 70.33 |
| | ATOM | 1787 | O | MET | 528 | 42.170 | -4.602 | 21.513 | 1.00 | 72.43 |
| | ATOM | 1788 | N | LYS | 529 | 42.834 | -2.739 | 20.428 | 1.00 | 71.53 |
| 40 | ATOM | 1789 | CA | LYS | 529 | 42.274 | -3.122 | 19.136 | 1.00 | 72.00 |
| | ATOM | 1790 | CB | LYS | 529 | 42.508 | -2.004 | 18.119 | 1.00 | 71.30 |
| | ATOM | 1791 | C | LYS | 529 | 42.813 | -4.439 | 18.587 | 1.00 | 72.47 |
| | ATOM | 1792 | O | LYS | 529 | 43.990 | -4.762 | 18.751 | 1.00 | 70.37 |
| | ATOM | 1793 | N | CYS | 530 | 41.932 | -5.191 | 17.930 | 1.00 | 74.48 |
| 45 | ATOM | 1794 | CA | CYS | 530 | 42.279 | -6.474 | 17.325 | 1.00 | 76.67 |
| | ATOM | 1795 | CB | CYS | 530 | 41.004 | -7.245 | 16.952 | 1.00 | 77.23 |
| | ATOM | 1796 | SG | CYS | 530 | 40.447 | -8.491 | 18.146 | 1.00 | 79.38 |
| | ATOM | 1797 | C | CYS | 530 | 43.098 | -6.220 | 16.065 | 1.00 | 78.08 |
| | ATOM | 1798 | O | CYS | 530 | 43.241 | -5.076 | 15.623 | 1.00 | 78.81 |
| 50 | ATOM | 1799 | N | LYS | 531 | 43.637 | -7.289 | 15.487 | 1.00 | 78.22 |
| | ATOM | 1800 | CA | LYS | 531 | 44.424 | -7.187 | 14.267 | 1.00 | 78.15 |
| | ATOM | 1801 | CB | LYS | 531 | 45.600 | -8.182 | 14.305 | 1.00 | 78.33 |
| | ATOM | 1802 | C | LYS | 531 | 43.508 | -7.467 | 13.067 | 1.00 | 77.93 |
| | ATOM | 1803 | O | LYS | 531 | 42.549 | -6.734 | 12.839 | 1.00 | 78.07 |
| 55 | ATOM | 1804 | N | ASN | 532 | 43.784 | -8.539 | 12.328 | 1.00 | 77.80 |
| | ATOM | 1805 | CA | ASN | 532 | 42.984 | -8.902 | 11.152 | 1.00 | 77.30 |
| | ATOM | 1806 | CB | ASN | 532 | 43.550 | -10.166 | 10.521 | 1.00 | 77.55 |
| | ATOM | 1807 | C | ASN | 532 | 41.485 | -9.082 | 11.423 | 1.00 | 77.34 |
| | ATOM | 1808 | O | ASN | 532 | 40.904 | -10.123 | 11.118 | 1.00 | 78.13 |
| 60 | ATOM | 1809 | N | VAL | 533 | 40.859 | -8.055 | 11.988 | 1.00 | 76.13 |
| | ATOM | 1810 | CA | VAL | 533 | 39.436 | -8.098 | 12.280 | 1.00 | 73.77 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1811 | CB | VAL | 533 | 39.155 | -7.715 | 13.752 | 1.00 | 73.62 |
| | ATOM | 1812 | CG1 | VAL | 533 | 39.690 | -6.327 | 14.047 | 1.00 | 73.13 |
| | ATOM | 1813 | CG2 | VAL | 533 | 37.662 | -7.782 | 14.021 | 1.00 | 73.14 |
| | ATOM | 1814 | C | VAL | 533 | 38.685 | -7.143 | 11.352 | 1.00 | 72.97 |
| | ATOM | 1815 | O | VAL | 533 | 39.024 | -5.960 | 11.252 | 1.00 | 73.91 |
| 10 | ATOM | 1816 | N | VAL | 534 | 37.671 | -7.666 | 10.666 | 1.00 | 70.02 |
| | ATOM | 1817 | CA | VAL | 534 | 36.866 | -6.867 | 9.747 | 1.00 | 66.70 |
| | ATOM | 1818 | CB | VAL | 534 | 35.619 | -7.646 | 9.328 | 1.00 | 67.32 |
| | ATOM | 1819 | C | VAL | 534 | 36.463 | -5.541 | 10.393 | 1.00 | 63.87 |
| | ATOM | 1820 | O | VAL | 534 | 35.895 | -5.519 | 11.486 | 1.00 | 63.55 |
| 15 | ATOM | 1821 | N | PRO | 535 | 36.756 | -4.415 | 9.719 | 1.00 | 60.92 |
| | ATOM | 1822 | CD | PRO | 535 | 37.424 | -4.354 | 8.408 | 1.00 | 61.01 |
| | ATOM | 1823 | CA | PRO | 535 | 36.424 | -3.077 | 10.229 | 1.00 | 56.83 |
| | ATOM | 1824 | CB | PRO | 535 | 36.867 | -2.135 | 9.107 | 1.00 | 58.70 |
| | ATOM | 1825 | CG | PRO | 535 | 37.023 | -3.009 | 7.893 | 1.00 | 61.55 |
| 20 | ATOM | 1826 | C | PRO | 535 | 34.944 | -2.902 | 10.571 | 1.00 | 52.90 |
| | ATOM | 1827 | O | PRO | 535 | 34.067 | -3.461 | 9.908 | 1.00 | 52.01 |
| | ATOM | 1828 | N | LEU | 536 | 34.672 | -2.120 | 11.610 | 1.00 | 48.60 |
| | ATOM | 1829 | CA | LEU | 536 | 33.301 | -1.874 | 12.042 | 1.00 | 45.08 |
| | ATOM | 1830 | CB | LEU | 536 | 33.280 | -0.796 | 13.128 | 1.00 | 44.35 |
| 25 | ATOM | 1831 | CG | LEU | 536 | 32.267 | -0.911 | 14.273 | 1.00 | 43.48 |
| | ATOM | 1832 | CD1 | LEU | 536 | 31.919 | 0.490 | 14.745 | 1.00 | 43.41 |
| | ATOM | 1833 | CD2 | LEU | 536 | 31.022 | -1.654 | 13.835 | 1.00 | 39.55 |
| | ATOM | 1834 | C | LEU | 536 | 32.434 | -1.433 | 10.871 | 1.00 | 43.58 |
| | ATOM | 1835 | O | LEU | 536 | 31.287 | -1.862 | 10.734 | 1.00 | 42.14 |
| 30 | ATOM | 1836 | N | TYR | 537 | 32.992 | -0.575 | 10.024 | 1.00 | 43.02 |
| | ATOM | 1837 | CA | TYR | 537 | 32.269 | -0.066 | 8.866 | 1.00 | 43.34 |
| | ATOM | 1838 | CB | TYR | 537 | 33.200 | 0.786 | 7.997 | 1.00 | 44.76 |
| | ATOM | 1839 | CG | TYR | 537 | 32.483 | 1.558 | 6.913 | 1.00 | 48.28 |
| | ATOM | 1840 | CD1 | TYR | 537 | 32.190 | 0.964 | 5.687 | 1.00 | 48.46 |
| 35 | ATOM | 1841 | CE1 | TYR | 537 | 31.504 | 1.660 | 4.693 | 1.00 | 52.48 |
| | ATOM | 1842 | CD2 | TYR | 537 | 32.073 | 2.875 | 7.123 | 1.00 | 49.99 |
| | ATOM | 1843 | CE2 | TYR | 537 | 31.383 | 3.584 | 6.135 | 1.00 | 53.73 |
| | ATOM | 1844 | CZ | TYR | 537 | 31.100 | 2.967 | 4.924 | 1.00 | 54.01 |
| | ATOM | 1845 | OH | TYR | 537 | 30.401 | 3.648 | 3.952 | 1.00 | 55.90 |
| 40 | ATOM | 1846 | C | TYR | 537 | 31.683 | -1.199 | 8.032 | 1.00 | 43.15 |
| | ATOM | 1847 | O | TYR | 537 | 30.500 | -1.191 | 7.696 | 1.00 | 41.54 |
| | ATOM | 1848 | N | ASP | 538 | 32.521 | -2.175 | 7.702 | 1.00 | 44.67 |
| | ATOM | 1849 | CA | ASP | 538 | 32.097 | -3.309 | 6.893 | 1.00 | 45.49 |
| | ATOM | 1850 | CB | ASP | 538 | 33.322 | -4.126 | 6.479 | 1.00 | 51.32 |
| 45 | ATOM | 1851 | CG | ASP | 538 | 34.361 | -3.284 | 5.748 | 1.00 | 56.17 |
| | ATOM | 1852 | OD1 | ASP | 538 | 35.436 | -3.820 | 5.396 | 1.00 | 57.29 |
| | ATOM | 1853 | OD2 | ASP | 538 | 34.097 | -2.079 | 5.526 | 1.00 | 59.24 |
| | ATOM | 1854 | C | ASP | 538 | 31.071 | -4.195 | 7.587 | 1.00 | 43.48 |
| | ATOM | 1855 | O | ASP | 538 | 30.177 | -4.738 | 6.940 | 1.00 | 43.95 |
| 50 | ATOM | 1856 | N | LEU | 539 | 31.193 | -4.345 | 8.901 | 1.00 | 41.57 |
| | ATOM | 1857 | CA | LEU | 539 | 30.244 | -5.157 | 9.654 | 1.00 | 39.11 |
| | ATOM | 1858 | CB | LEU | 539 | 30.734 | -5.351 | 11.092 | 1.00 | 41.88 |
| | ATOM | 1859 | CG | LEU | 539 | 29.770 | -6.065 | 12.044 | 1.00 | 46.11 |
| | ATOM | 1860 | CD1 | LEU | 539 | 29.298 | -7.379 | 11.423 | 1.00 | 46.99 |
| 55 | ATOM | 1861 | CD2 | LEU | 539 | 30.474 | -6.319 | 13.377 | 1.00 | 45.76 |
| | ATOM | 1862 | C | LEU | 539 | 28.891 | -4.451 | 9.651 | 1.00 | 36.38 |
| | ATOM | 1863 | O | LEU | 539 | 27.849 | -5.070 | 9.436 | 1.00 | 35.74 |
| | ATOM | 1864 | N | LEU | 540 | 28.919 | -3.146 | 9.894 | 1.00 | 35.50 |
| | ATOM | 1865 | CA | LEU | 540 | 27.703 | -2.336 | 9.903 | 1.00 | 35.59 |
| 60 | ATOM | 1866 | CB | LEU | 540 | 28.061 | -0.877 | 10.219 | 1.00 | 37.63 |
| | ATOM | 1867 | CG | LEU | 540 | 27.856 | -0.252 | 11.605 | 1.00 | 40.28 |

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|----|------|------|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 1868 | CD1 | LEU | 540 | 27.526 | -1.299 | 12.645 | 1.00 | 38.55 |
| | ATOM | 1869 | CD2 | LEU | 540 | 29.114 | 0.506 | 11.985 | 1.00 | 41.04 |
| | ATOM | 1870 | C | LEU | 540 | 27.060 | -2.415 | 8.510 | 1.00 | 35.50 |
| | ATOM | 1871 | O | LEU | 540 | 25.846 | -2.585 | 8.371 | 1.00 | 33.21 |
| 10 | ATOM | 1872 | N | LEU | 541 | 27.892 | -2.289 | 7.483 | 1.00 | 37.01 |
| | ATOM | 1873 | CA | LEU | 541 | 27.418 | -2.340 | 6.101 | 1.00 | 38.51 |
| | ATOM | 1874 | CB | LEU | 541 | 28.591 | -2.152 | 5.145 | 1.00 | 39.67 |
| | ATOM | 1875 | CG | LEU | 541 | 28.301 | -2.112 | 3.643 | 1.00 | 40.92 |
| 15 | ATOM | 1876 | CD1 | LEU | 541 | 27.184 | -1.130 | 3.348 | 1.00 | 42.44 |
| | ATOM | 1877 | CD2 | LEU | 541 | 29.572 | -1.716 | 2.908 | 1.00 | 44.18 |
| | ATOM | 1878 | C | LEU | 541 | 26.723 | -3.676 | 5.833 | 1.00 | 39.75 |
| | ATOM | 1879 | O | LEU | 541 | 25.616 | -3.713 | 5.297 | 1.00 | 36.48 |
| 20 | ATOM | 1880 | N | GLU | 542 | 27.366 | -4.770 | 6.230 | 1.00 | 40.88 |
| | ATOM | 1881 | CA | GLU | 542 | 26.790 | -6.097 | 6.037 | 1.00 | 41.89 |
| | ATOM | 1882 | CB | GLU | 542 | 27.719 | -7.170 | 6.620 | 1.00 | 44.11 |
| | ATOM | 1883 | CG | GLU | 542 | 27.010 | -8.457 | 7.052 | 1.00 | 50.60 |
| 25 | ATOM | 1884 | CD | GLU | 542 | 26.434 | -9.245 | 5.887 | 1.00 | 55.80 |
| | ATOM | 1885 | OE1 | GLU | 542 | 25.570 | -10.117 | 6.130 | 1.00 | 58.81 |
| | ATOM | 1886 | OE2 | GLU | 542 | 26.842 | -8.996 | 4.728 | 1.00 | 57.19 |
| | ATOM | 1887 | C | GLU | 542 | 25.414 | -6.195 | 6.691 | 1.00 | 41.58 |
| 30 | ATOM | 1888 | O | GLU | 542 | 24.472 | -6.720 | 6.102 | 1.00 | 42.82 |
| | ATOM | 1889 | N | MET | 543 | 25.298 | -5.686 | 7.915 | 1.00 | 40.09 |
| | ATOM | 1890 | CA | MET | 543 | 24.036 | -5.731 | 8.634 | 1.00 | 36.43 |
| | ATOM | 1891 | CB | MET | 543 | 24.270 | -5.424 | 10.111 | 1.00 | 39.95 |
| 35 | ATOM | 1892 | CG | MET | 543 | 25.137 | -6.459 | 10.808 | 1.00 | 41.95 |
| | ATOM | 1893 | SD | MET | 543 | 24.918 | -6.445 | 12.604 | 1.00 | 47.17 |
| | ATOM | 1894 | CE | MET | 543 | 25.324 | -4.749 | 12.964 | 1.00 | 40.88 |
| | ATOM | 1895 | C | MET | 543 | 23.001 | -4.769 | 8.072 | 1.00 | 35.02 |
| 40 | ATOM | 1896 | O | MET | 543 | 21.808 | -5.073 | 8.048 | 1.00 | 35.31 |
| | ATOM | 1897 | N | LEU | 544 | 23.457 | -3.605 | 7.629 | 1.00 | 32.90 |
| | ATOM | 1898 | CA | LEU | 544 | 22.559 | -2.603 | 7.074 | 1.00 | 36.88 |
| | ATOM | 1899 | CB | LEU | 544 | 23.225 | -1.226 | 7.111 | 1.00 | 34.51 |
| 45 | ATOM | 1900 | CG | LEU | 544 | 23.268 | -0.562 | 8.490 | 1.00 | 31.94 |
| | ATOM | 1901 | CD1 | LEU | 544 | 24.284 | 0.564 | 8.478 | 1.00 | 32.27 |
| | ATOM | 1902 | CD2 | LEU | 544 | 21.897 | -0.029 | 8.846 | 1.00 | 29.02 |
| | ATOM | 1903 | C | LEU | 544 | 22.148 | -2.941 | 5.640 | 1.00 | 38.94 |
| 50 | ATOM | 1904 | O | LEU | 544 | 20.971 | -2.842 | 5.294 | 1.00 | 39.52 |
| | ATOM | 1905 | N | ASP | 545 | 23.118 | -3.338 | 4.817 | 1.00 | 41.05 |
| | ATOM | 1906 | CA | ASP | 545 | 22.850 | -3.685 | 3.418 | 1.00 | 40.78 |
| | ATOM | 1907 | CB | ASP | 545 | 24.159 | -3.780 | 2.620 | 1.00 | 37.75 |
| 55 | ATOM | 1908 | CG | ASP | 545 | 23.922 | -3.937 | 1.120 | 1.00 | 35.19 |
| | ATOM | 1909 | OD1 | ASP | 545 | 24.881 | -4.265 | 0.380 | 1.00 | 33.48 |
| | ATOM | 1910 | OD2 | ASP | 545 | 22.768 | -3.734 | 0.691 | 1.00 | 31.33 |
| | ATOM | 1911 | C | ASP | 545 | 22.116 | -5.015 | 3.349 | 1.00 | 42.87 |
| 60 | ATOM | 1912 | O | ASP | 545 | 22.681 | -6.030 | 2.929 | 1.00 | 44.32 |
| | ATOM | 1913 | N | ALA | 546 | 20.853 | -5.009 | 3.755 | 1.00 | 43.49 |
| | ATOM | 1914 | CA | ALA | 546 | 20.069 | -6.229 | 3.746 | 1.00 | 46.96 |
| | ATOM | 1915 | CB | ALA | 546 | 19.213 | -6.305 | 5.006 | 1.00 | 47.82 |
| 65 | ATOM | 1916 | C | ALA | 546 | 19.193 | -6.362 | 2.508 | 1.00 | 49.55 |
| | ATOM | 1917 | O | ALA | 546 | 18.804 | -5.368 | 1.883 | 1.00 | 48.75 |
| | ATOM | 1918 | N | HIS | 547 | 18.895 | -7.606 | 2.152 | 1.00 | 50.98 |
| | ATOM | 1919 | CA | HIS | 547 | 18.042 | -7.884 | 1.006 | 1.00 | 53.77 |
| 70 | ATOM | 1920 | CB | HIS | 547 | 18.431 | -9.223 | 0.369 | 1.00 | 52.69 |
| | ATOM | 1921 | CG | HIS | 547 | 18.395 | -10.382 | 1.317 | 1.00 | 55.05 |
| | ATOM | 1922 | CD2 | HIS | 547 | 17.477 | -10.752 | 2.242 | 1.00 | 53.94 |
| | ATOM | 1923 | ND1 | HIS | 547 | 19.395 | -11.329 | 1.371 | 1.00 | 56.23 |
| | ATOM | 1924 | CE1 | HIS | 547 | 19.095 | -12.232 | 2.286 | 1.00 | 55.36 |

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|----|--------|------|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 1925 | NE2 | HIS | 547 | 17.936 | -11.906 | 2.830 | 1.00 | 57.01 |
| | ATOM | 1926 | C | HIS | 547 | 16.603 | -7.936 | 1.518 | 1.00 | 55.69 |
| | ATOM | 1927 | O | HIS | 547 | 16.362 | -7.796 | 2.720 | 1.00 | 54.30 |
| | ATOM | 1928 | N | ARG | 548 | 15.653 | -8.139 | 0.612 | 1.00 | 57.00 |
| | ATOM | 1929 | CA | ARG | 548 | 14.245 | -8.212 | 0.987 | 1.00 | 60.65 |
| 10 | ATOM | 1930 | CB | ARG | 548 | 13.432 | -7.171 | 0.208 | 1.00 | 62.69 |
| | ATOM | 1931 | CG | ARG | 548 | 14.272 | -6.222 | -0.637 | 1.00 | 67.54 |
| | ATOM | 1932 | CD | ARG | 548 | 13.448 | -5.061 | -1.171 | 1.00 | 71.92 |
| | ATOM | 1933 | NE | ARG | 548 | 13.702 | -3.826 | -0.432 | 1.00 | 76.95 |
| | ATOM | 1934 | CZ | ARG | 548 | 14.864 | -3.178 | -0.429 | 1.00 | 79.04 |
| 15 | ATOM | 1935 | NH1 | ARG | 548 | 15.891 | -3.644 | -1.128 | 1.00 | 80.66 |
| | ATOM | 1936 | NH2 | ARG | 548 | 15.001 | -2.063 | 0.278 | 1.00 | 80.39 |
| | ATOM | 1937 | C | ARG | 548 | 13.695 | -9.608 | 0.711 | 1.00 | 61.65 |
| | ATOM | 1938 | O | ARG | 548 | 12.500 | -9.781 | 0.466 | 1.00 | 62.05 |
| | ATOM | 1939 | N | LEU | 549 | 14.576 | -10.603 | 0.756 | 1.00 | 62.39 |
| 20 | ATOM | 1940 | CA | LEU | 549 | 14.188 | -11.985 | 0.507 | 1.00 | 64.02 |
| | ATOM | 1941 | CB | LEU | 549 | 15.433 | -12.828 | 0.195 | 1.00 | 62.14 |
| | ATOM | 1942 | CG | LEU | 549 | 16.461 | -12.191 | -0.753 | 1.00 | 60.76 |
| | ATOM | 1943 | CD1 | LEU | 549 | 17.699 | -13.074 | -0.878 | 1.00 | 57.77 |
| | ATOM | 1944 | CD2 | LEU | 549 | 15.823 | -11.972 | -2.108 | 1.00 | 58.38 |
| 25 | ATOM | 1945 | C | LEU | 549 | 13.431 | -12.574 | 1.702 | 1.00 | 66.65 |
| | ATOM | 1946 | O | LEU | 549 | 12.759 | -13.600 | 1.577 | 1.00 | 67.15 |
| | ATOM | 1947 | N | HIS | 550 | 13.541 | -11.920 | 2.856 | 1.00 | 67.72 |
| | ATOM | 1948 | CA | HIS | 550 | 12.858 | -12.378 | 4.065 | 1.00 | 69.93 |
| | ATOM | 1949 | CB | HIS | 550 | 13.753 | -12.190 | 5.298 | 1.00 | 70.76 |
| 30 | ATOM | 1950 | CG | HIS | 550 | 14.977 | -13.054 | 5.306 | 1.00 | 71.50 |
| | ATOM | 1951 | CD2 | HIS | 550 | 15.539 | -13.821 | 4.341 | 1.00 | 71.63 |
| | ATOM | 1952 | ND1 | HIS | 550 | 15.793 | -13.172 | 6.411 | 1.00 | 71.98 |
| | ATOM | 1953 | CE1 | HIS | 550 | 16.805 | -13.972 | 6.126 | 1.00 | 72.04 |
| | ATOM | 1954 | NE2 | HIS | 550 | 16.674 | -14.379 | 4.876 | 1.00 | 71.39 |
| 35 | ATOM | 1955 | C | HIS | 550 | 11.556 | -11.603 | 4.275 | 1.00 | 71.15 |
| | ATOM | 1956 | O | HIS | 550 | 10.940 | -11.684 | 5.340 | 1.00 | 70.66 |
| | ATOM | 1957 | N | ALA | 551 | 11.143 | -10.851 | 3.258 | 1.00 | 72.22 |
| | ATOM | 1958 | CA | ALA | 551 | 9.919 | -10.057 | 3.338 | 1.00 | 73.58 |
| | ATOM | 1959 | CB | ALA | 551 | 9.904 | -9.014 | 2.221 | 1.00 | 73.21 |
| 40 | ATOM | 1960 | C | ALA | 551 | 8.658 | -10.920 | 3.266 | 1.00 | 74.69 |
| | ATOM | 1961 | O | ALA | 551 | 7.684 | -10.474 | 2.621 | 1.00 | 76.12 |
| | ATOM | 1962 | OXT | ALA | 551 | 8.651 | -12.025 | 3.852 | 1.00 | 73.79 |
| | HETATM | 1963 | C10 | OHT | 600 | 30.581 | 1.481 | 29.471 | 1.00 | 26.84 |
| | HETATM | 1964 | C9 | OHT | 600 | 30.713 | -0.043 | 29.358 | 1.00 | 22.85 |
| 45 | HETATM | 1965 | C8 | OHT | 600 | 31.366 | -0.385 | 28.037 | 1.00 | 25.56 |
| | HETATM | 1966 | C11 | OHT | 600 | 32.761 | 0.051 | 27.916 | 1.00 | 27.51 |
| | HETATM | 1967 | C16 | OHT | 600 | 33.218 | 0.797 | 26.797 | 1.00 | 28.35 |
| | HETATM | 1968 | C15 | OHT | 600 | 34.551 | 1.237 | 26.747 | 1.00 | 30.39 |
| | HETATM | 1969 | C14 | OHT | 600 | 35.443 | 0.923 | 27.792 | 1.00 | 30.23 |
| 50 | HETATM | 1970 | C13 | OHT | 600 | 35.004 | 0.185 | 28.890 | 1.00 | 31.45 |
| | HETATM | 1971 | C12 | OHT | 600 | 33.666 | -0.241 | 28.955 | 1.00 | 27.93 |
| | HETATM | 1972 | C7 | OHT | 600 | 30.682 | -1.089 | 27.077 | 1.00 | 24.41 |
| | HETATM | 1973 | C1 | OHT | 600 | 29.211 | -1.258 | 27.052 | 1.00 | 24.26 |
| | HETATM | 1974 | C2 | OHT | 600 | 28.644 | -2.526 | 26.706 | 1.00 | 25.92 |
| 55 | HETATM | 1975 | C3 | OHT | 600 | 27.254 | -2.668 | 26.580 | 1.00 | 26.32 |
| | HETATM | 1976 | C4 | OHT | 600 | 26.438 | -1.553 | 26.813 | 1.00 | 29.02 |
| | HETATM | 1977 | O4 | OHT | 600 | 25.072 | -1.605 | 26.716 | 1.00 | 28.42 |
| | HETATM | 1978 | C5 | OHT | 600 | 26.980 | -0.286 | 27.130 | 1.00 | 26.98 |
| | HETATM | 1979 | C6 | OHT | 600 | 28.362 | -0.147 | 27.231 | 1.00 | 25.23 |
| 60 | HETATM | 1980 | C17 | OHT | 600 | 31.370 | -1.692 | 25.942 | 1.00 | 26.61 |
| | HETATM | 1981 | C18 | OHT | 600 | 32.508 | -2.498 | 26.151 | 1.00 | 26.77 |

| | | | | | | | | | | |
|----|--------|------|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | HETATM | 1982 | C19 | OHT | 600 | 33.166 | -3.052 | 25.072 | 1.00 | 27.50 |
| | HETATM | 1983 | C20 | OHT | 600 | 32.676 | -2.794 | 23.786 | 1.00 | 27.50 |
| | HETATM | 1984 | O20 | OHT | 600 | 33.206 | -3.566 | 22.795 | 1.00 | 31.35 |
| | HETATM | 1985 | C23 | OHT | 600 | 33.009 | -3.135 | 21.448 | 1.00 | 40.09 |
| | HETATM | 1986 | C24 | OHT | 600 | 34.226 | -3.490 | 20.575 | 1.00 | 44.80 |
| 10 | HETATM | 1987 | N24 | OHT | 600 | 34.141 | -4.901 | 20.203 | 1.00 | 49.00 |
| | HETATM | 1988 | C25 | OHT | 600 | 33.375 | -5.040 | 18.933 | 1.00 | 51.64 |
| | HETATM | 1989 | C26 | OHT | 600 | 35.495 | -5.459 | 20.004 | 1.00 | 52.06 |
| | HETATM | 1990 | C21 | OHT | 600 | 31.540 | -2.005 | 23.558 | 1.00 | 27.19 |
| | HETATM | 1991 | C22 | OHT | 600 | 30.892 | -1.450 | 24.645 | 1.00 | 27.92 |
| 15 | HETATM | 1992 | O1 | HOH | 1 | 20.714 | -12.010 | 23.057 | 1.00 | 27.20 |
| | HETATM | 1993 | O1 | HOH | 2 | 22.563 | -0.070 | 25.819 | 1.00 | 25.77 |
| | HETATM | 1994 | O1 | HOH | 3 | 25.183 | 19.202 | 23.149 | 1.00 | 42.52 |
| | HETATM | 1995 | O1 | HOH | 4 | 35.158 | 5.823 | 37.390 | 1.00 | 33.92 |
| | HETATM | 1996 | O1 | HOH | 5 | 22.116 | -9.922 | 18.914 | 1.00 | 30.18 |
| 20 | HETATM | 1997 | O1 | HOH | 6 | 29.812 | 6.536 | 19.652 | 1.00 | 26.11 |
| | HETATM | 1998 | O1 | HOH | 7 | 13.362 | 4.463 | 20.376 | 1.00 | 29.40 |
| | HETATM | 1999 | O1 | HOH | 8 | 19.799 | -11.295 | 20.187 | 1.00 | 28.70 |
| | HETATM | 2000 | O1 | HOH | 9 | 21.205 | 1.466 | 23.794 | 1.00 | 22.47 |
| | HETATM | 2001 | O1 | HOH | 10 | 21.177 | -4.961 | 29.066 | 1.00 | 33.00 |
| 25 | HETATM | 2002 | O1 | HOH | 11 | 18.591 | 1.863 | 20.518 | 1.00 | 32.59 |
| | HETATM | 2003 | O1 | HOH | 12 | 16.298 | 21.566 | 15.992 | 1.00 | 33.42 |
| | HETATM | 2004 | O1 | HOH | 13 | 18.611 | 1.976 | 24.494 | 1.00 | 29.70 |
| | HETATM | 2005 | O1 | HOH | 14 | 38.009 | 8.910 | 21.156 | 1.00 | 39.92 |
| | HETATM | 2006 | O1 | HOH | 15 | 26.549 | 11.664 | 18.080 | 1.00 | 30.25 |
| 30 | HETATM | 2007 | O1 | HOH | 16 | 20.282 | -4.239 | 26.512 | 1.00 | 32.70 |
| | HETATM | 2008 | O1 | HOH | 17 | 32.858 | 8.754 | 20.237 | 1.00 | 29.88 |
| | HETATM | 2009 | O1 | HOH | 18 | 8.497 | 16.136 | 29.934 | 1.00 | 46.80 |
| | HETATM | 2010 | O1 | HOH | 19 | 21.940 | 19.301 | 31.632 | 1.00 | 35.72 |
| | HETATM | 2011 | O1 | HOH | 20 | 35.153 | 2.682 | 14.122 | 1.00 | 41.02 |
| 35 | HETATM | 2012 | O1 | HOH | 21 | 20.358 | -2.268 | 21.013 | 1.00 | 29.43 |
| | HETATM | 2013 | O1 | HOH | 22 | 35.562 | 10.036 | 36.334 | 1.00 | 41.37 |
| | HETATM | 2014 | O1 | HOH | 23 | 17.248 | 18.187 | 17.571 | 1.00 | 33.96 |
| | HETATM | 2015 | O1 | HOH | 24 | 18.445 | 20.973 | 12.346 | 1.00 | 43.44 |
| | HETATM | 2016 | O1 | HOH | 25 | 12.152 | 23.054 | 33.132 | 1.00 | 36.04 |
| 40 | HETATM | 2017 | O1 | HOH | 26 | 13.181 | 22.222 | 9.699 | 1.00 | 37.03 |
| | HETATM | 2018 | O1 | HOH | 27 | 19.399 | -6.090 | 12.808 | 1.00 | 44.86 |
| | HETATM | 2019 | O1 | HOH | 28 | 37.895 | 13.599 | 31.395 | 1.00 | 47.26 |
| | HETATM | 2020 | O1 | HOH | 29 | 11.570 | 6.212 | 7.962 | 1.00 | 51.10 |
| | HETATM | 2021 | O1 | HOH | 30 | 20.172 | -2.568 | 23.445 | 1.00 | 51.70 |
| 45 | HETATM | 2022 | O1 | HOH | 31 | 36.402 | -5.369 | 23.729 | 1.00 | 58.20 |
| | HETATM | 2023 | O1 | HOH | 32 | 25.127 | 13.802 | 19.187 | 1.00 | 35.29 |
| | HETATM | 2024 | O1 | HOH | 33 | 23.181 | 4.937 | 38.538 | 1.00 | 33.77 |
| | HETATM | 2025 | O1 | HOH | 34 | 20.550 | 0.421 | 21.276 | 1.00 | 29.12 |
| | HETATM | 2026 | O1 | HOH | 35 | 39.599 | 13.954 | 27.312 | 1.00 | 44.08 |
| 50 | HETATM | 2027 | O1 | HOH | 36 | 26.445 | 13.863 | 21.285 | 1.00 | 34.97 |
| | HETATM | 2028 | O1 | HOH | 37 | 13.759 | 5.079 | 9.108 | 1.00 | 38.54 |
| | HETATM | 2029 | O1 | HOH | 38 | 14.150 | 24.731 | 34.529 | 1.00 | 49.72 |
| | HETATM | 2030 | O1 | HOH | 39 | 21.060 | 13.886 | -6.319 | 1.00 | 59.79 |
| | HETATM | 2031 | O1 | HOH | 40 | 32.215 | 6.217 | 8.726 | 1.00 | 60.22 |
| 55 | HETATM | 2032 | O1 | HOH | 41 | 35.105 | 15.704 | 9.069 | 1.00 | 45.15 |
| | HETATM | 2033 | O1 | HOH | 42 | 11.427 | 19.451 | 9.903 | 1.00 | 38.56 |
| | HETATM | 2034 | O1 | HOH | 43 | 19.662 | 23.472 | 10.333 | 1.00 | 47.71 |
| | HETATM | 2035 | O1 | HOH | 44 | 9.231 | 3.690 | 12.337 | 1.00 | 45.98 |
| | HETATM | 2036 | O1 | HOH | 45 | 15.313 | -6.036 | 17.192 | 1.00 | 39.07 |
| 60 | HETATM | 2037 | O1 | HOH | 46 | 15.517 | -3.266 | 17.907 | 1.00 | 37.67 |
| | HETATM | 2038 | O1 | HOH | 47 | 28.784 | -16.713 | 25.163 | 1.00 | 55.44 |

| | | | | | | | | | | |
|----|--------|------|----|-----|----|--------|---------|--------|------|-------|
| 5 | HETATM | 2039 | 01 | HOH | 48 | 27.868 | -10.898 | 28.271 | 1.00 | 31.27 |
| | HETATM | 2040 | 01 | HOH | 49 | 6.955 | 13.568 | 28.233 | 1.00 | 48.83 |
| | HETATM | 2041 | 01 | HOH | 50 | 22.051 | -15.030 | 28.603 | 1.00 | 36.91 |
| | HETATM | 2042 | 01 | HOH | 51 | 7.026 | 31.002 | 30.284 | 1.00 | 46.73 |
| | HETATM | 2043 | 01 | HOH | 52 | -1.489 | 12.385 | 15.164 | 1.00 | 51.17 |
| 10 | HETATM | 2044 | 01 | HOH | 53 | 3.499 | 6.444 | 14.452 | 1.00 | 50.38 |
| | HETATM | 2045 | 01 | HOH | 54 | 18.655 | -2.048 | 25.518 | 1.00 | 52.29 |
| | HETATM | 2046 | 01 | HOH | 55 | 28.188 | -15.195 | 38.996 | 1.00 | 55.22 |
| | HETATM | 2047 | 01 | HOH | 56 | 35.275 | -10.556 | 38.061 | 1.00 | 57.39 |
| | HETATM | 2048 | 01 | HOH | 57 | 37.771 | -9.103 | 34.605 | 1.00 | 54.17 |
| 15 | HETATM | 2049 | 01 | HOH | 58 | 31.403 | -3.039 | 17.983 | 1.00 | 46.80 |
| | HETATM | 2050 | 01 | HOH | 59 | 30.455 | -6.352 | 17.005 | 1.00 | 47.05 |
| | HETATM | 2051 | 01 | HOH | 60 | 25.985 | 8.255 | 0.416 | 1.00 | 43.32 |
| | HETATM | 2052 | 01 | HOH | 61 | 35.679 | 0.749 | 10.462 | 1.00 | 42.99 |
| | HETATM | 2053 | 01 | HOH | 62 | 14.741 | 4.029 | 33.936 | 1.00 | 49.59 |
| 20 | HETATM | 2054 | 01 | HOH | 63 | 16.333 | 2.592 | 35.952 | 1.00 | 45.13 |
| | HETATM | 2055 | 01 | HOH | 64 | 23.809 | 7.186 | 39.798 | 1.00 | 45.36 |
| | HETATM | 2056 | 01 | HOH | 65 | 27.012 | -1.948 | 46.995 | 1.00 | 63.39 |
| | HETATM | 2057 | 01 | HOH | 66 | 25.956 | -6.422 | 42.144 | 1.00 | 44.94 |
| | HETATM | 2058 | 01 | HOH | 67 | 23.510 | -8.414 | 39.036 | 1.00 | 39.06 |
| 25 | HETATM | 2059 | 01 | HOH | 68 | 41.475 | 0.971 | 33.110 | 1.00 | 55.50 |
| | HETATM | 2060 | 01 | HOH | 69 | 36.519 | 8.863 | 38.836 | 1.00 | 41.56 |
| | HETATM | 2061 | 01 | HOH | 70 | 30.111 | 14.823 | 12.793 | 1.00 | 44.58 |
| | HETATM | 2062 | 01 | HOH | 71 | 26.850 | -6.092 | 1.594 | 1.00 | 40.15 |
| | HETATM | 2063 | 01 | HOH | 72 | 20.448 | -3.169 | 1.055 | 1.00 | 42.50 |
| 30 | HETATM | 2064 | 01 | HOH | 73 | 33.896 | 3.047 | 16.172 | 1.00 | 46.39 |
| | HETATM | 2065 | 01 | HOH | 74 | 16.884 | 0.446 | 26.043 | 1.00 | 61.50 |
| | HETATM | 2066 | 01 | HOH | 75 | 18.595 | 0.296 | 27.866 | 1.00 | 47.33 |
| | HETATM | 2067 | 01 | HOH | 76 | 6.166 | 21.439 | 19.124 | 1.00 | 47.94 |
| | HETATM | 2068 | 01 | HOH | 77 | 18.484 | 20.060 | 16.232 | 1.00 | 35.52 |
| 35 | HETATM | 2069 | 01 | HOH | 78 | 1.985 | 23.265 | 29.187 | 1.00 | 46.42 |
| | HETATM | 2070 | 01 | HOH | 79 | 12.729 | 30.461 | 27.530 | 1.00 | 62.79 |
| | END | | | | | | | | | |

5 Phe Lys Asn Leu Pro Leu Glu Asp Gln Ile Thr Leu Ile Gln Tyr Ser
 20 25 30

Trp

10

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Glu Phe Pro Ala Met Leu Val Glu Ile Ile Ser Asp

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Phe Arg Asn Leu His Val Asp Asp Gln Met Ala Val Ile Gln Tyr Ser

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Trp

35

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40 <212> PRT

<213> Homo sapiens

<400> 51

Asp Phe Pro Glu Met Met Ala Glu Ile Ile Ser Val

1

5

10

45

50

WHAT IS CLAIMED IS:

55 1. A method of identifying a compound that modulates coactivator binding to a nuclear receptor, said method comprising:

modeling test compounds that fit spacially into a nuclear receptor coactivator binding site of interest using an atomic structural model of a nuclear receptor coactivator binding site or portion thereof.

5 screening said test compounds in an assay characterized by binding of a test compound to a nuclear receptor coactivator binding site. and
identifying a test compound that modulates coactivator binding to said nuclear receptor.

10 2. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of Val284, Phe293, Ile302, Leu305, and Leu454.

15 3. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of Val284, Lys288, Ile302, Lys306, Leu454 and Glu457.

20 4. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.

25 5. The method of claim 1, wherein said nuclear receptor coactivator binding site comprises amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.

30 6. The method of claim 5, wherein said amino acid residues corresponding to residues of human thyroid receptor comprise Val284, Phe293, Ile302, Leu305, and Leu454.

35 7. The method of claim 5, wherein said amino acid residues corresponding to residues of human thyroid receptor comprise Val284, Lys288, Ile302, Lys306, Leu454 and Glu457.

8. The method of claim 1, wherein said nuclear receptor coactivator binding site comprises amino acid residues corresponding to residues of human thyroid receptor of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5

5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.

9. The method of any one of claims 5 through 8, wherein said nuclear receptor is selected from the group consisting of TR, RAR, RXR, PPAR, VDR, ER, GR, PR, MR, and AR.

10

10. The method of claim 1, wherein said screening is *in vitro*.

11. The method of claim 10, wherein said screening is high throughput screening.

15

12. The method of claim 1, wherein said assay is a biological assay.

13. The method of claim 1, wherein said test compound is from a library of compounds.

20

14. The method of claim 1, wherein said test compound is an agonist or antagonist of coactivator binding.

15. The method of claim 14, wherein said test compound is a small organic molecule, a peptide, or peptidomimetic.

25

16. The method of claim 15, wherein said compound is a peptide comprising a NR-box amino acid sequence, or derivative thereof.

17. A method for identifying an agonist or antagonist of coactivator binding to a nuclear receptor, said method comprising the steps of:

30

providing the atomic coordinates of a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system;

modeling compounds which fit spacially into the nuclear receptor coactivator binding site; and

35

identifying in an assay for nuclear receptor activity a compound that increases or decreases the activity of said nuclear receptor by binding the coactivator binding site of said nuclear receptor, whereby an agonist or antagonist of coactivator binding is identified.

5 18. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecular complex of a compound bound to a nuclear receptor coactivator binding site comprising structure coordinates of amino acids corresponding to human thyroid receptor amino acids selected
10 from the group consisting of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459, or a homologue of said molecular complex, wherein said homologue comprises a coactivator binding site that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

15

 19. The machine readable storage medium of claim 18, wherein said nuclear receptor is a thyroid receptor.

 20. The machine readable storage medium of claim 19, wherein said thyroid receptor is
20 human.

 21. The machine readable storage medium of claim 20, wherein said molecule is peptide.

 22. The machine readable storage medium of claim 21, wherein said peptide comprises a
25 NR-box amino acid sequence, or derivative thereof.

 23. The machine-readable data storage medium according to claim 18, wherein said molecular complex is defined by the set of structure coordinates depicted in Appendix 1, or a homologue of said molecular complex, said homologue having a root mean square deviation from
30 the backbone atoms of said amino acids of not more than 1.5Å.

 24. A machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data which, when combined with a second set of machine readable data, using a machine programmed with instructions for using said first set of data
35 and said second set of data, can determine at least a portion of the structure coordinates corresponding to the second set of machine readable data, wherein: said first set of data comprises a Fourier transform of at least a portion of the structural coordinates selected from the group

- 5 consisting of coordinates depicted in Appendix 1; and said second set of data comprises an X-ray diffraction pattern of a molecule or molecular complex.

25. A cocrystal of a nuclear receptor comprising a molecule bound to the coactivator binding site of said nuclear receptor.

10

26. The cocrystal of claim 25, wherein said nuclear receptor is a thyroid receptor.

27. The cocrystal of claim 26, wherein said thyroid receptor is human.

15

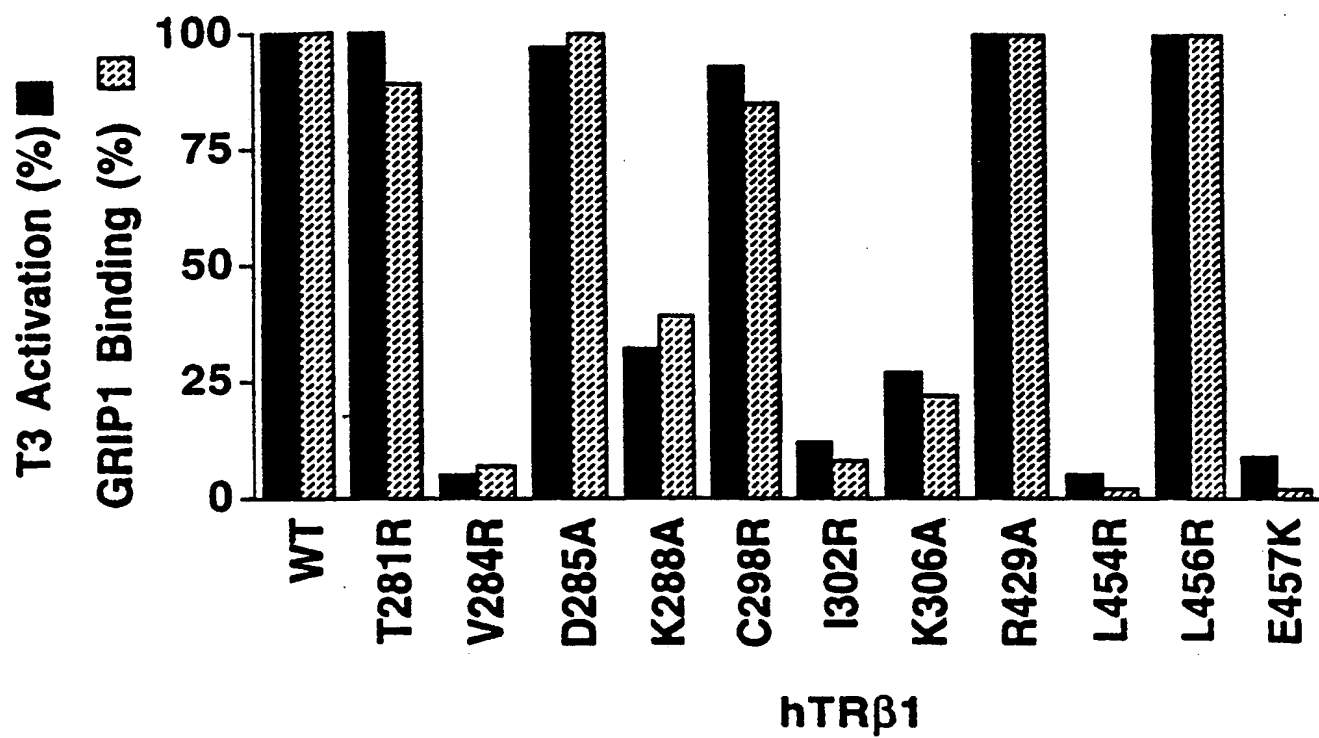
28. The cocrystal of claim 27, wherein said molecule is peptide.

29. The cocrystal of claim 28, wherein said peptide comprises a NR-box amino acid sequence or derivative thereof.

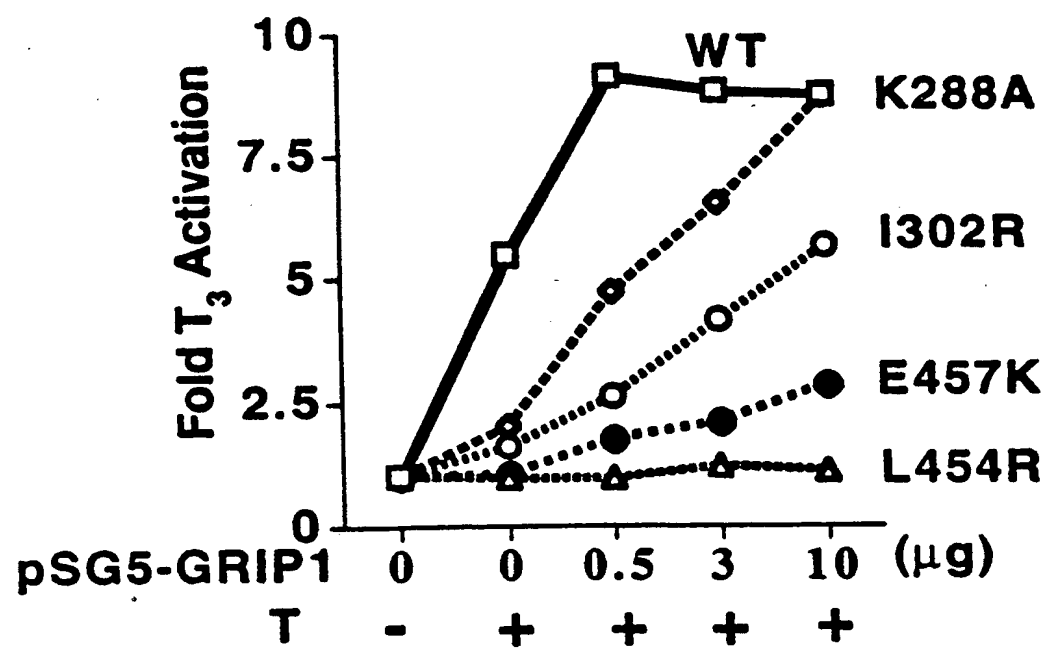
20

30. A compound identified according to the method of claim 1.

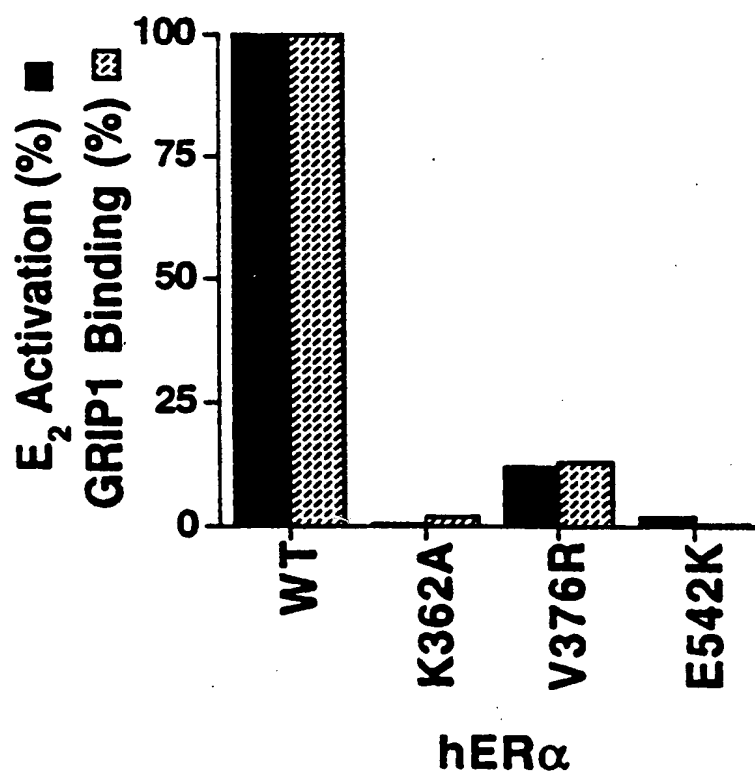
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FIGURE 1

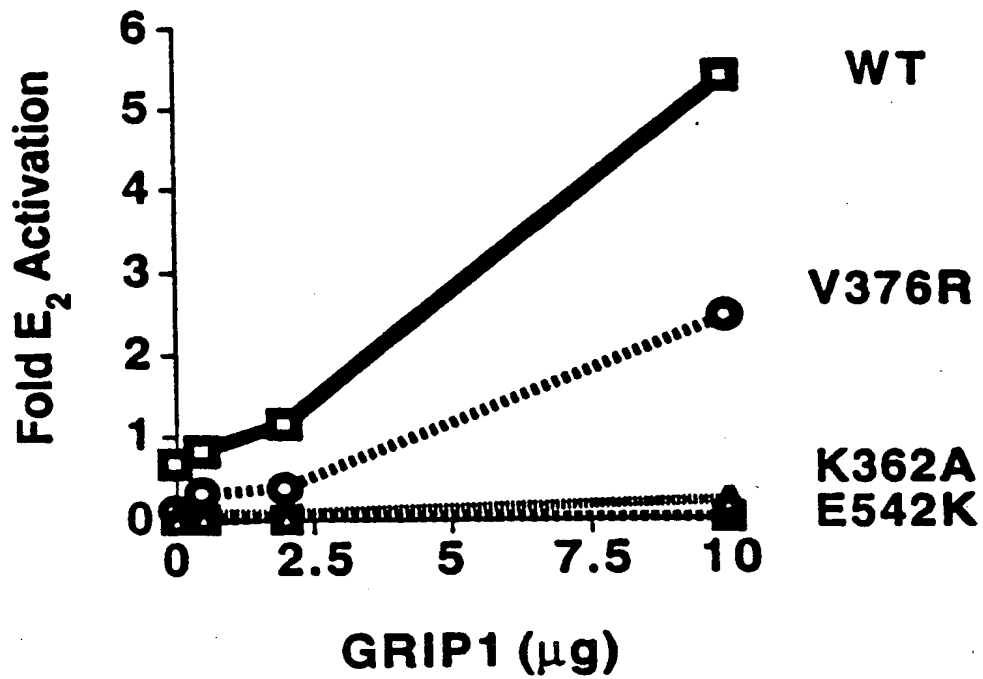
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FIGURE 2

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FIGURE 3

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FIGURE 4

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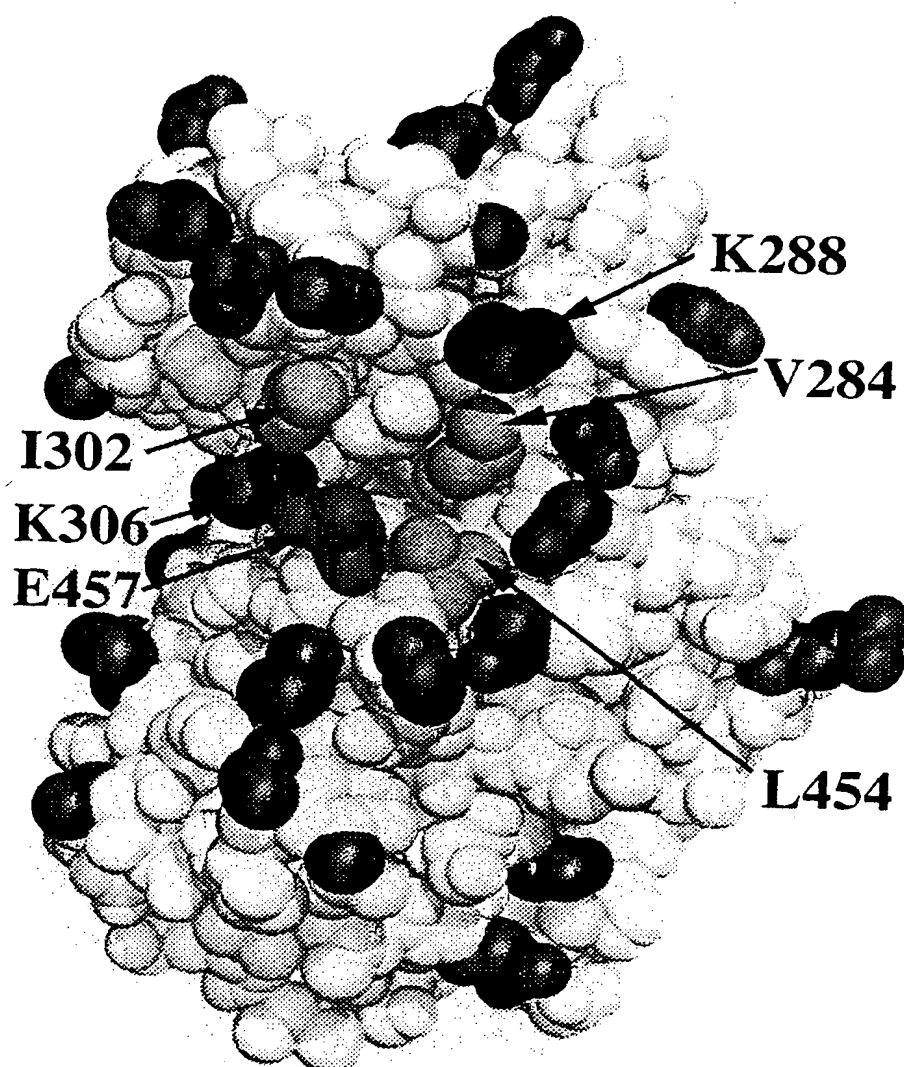
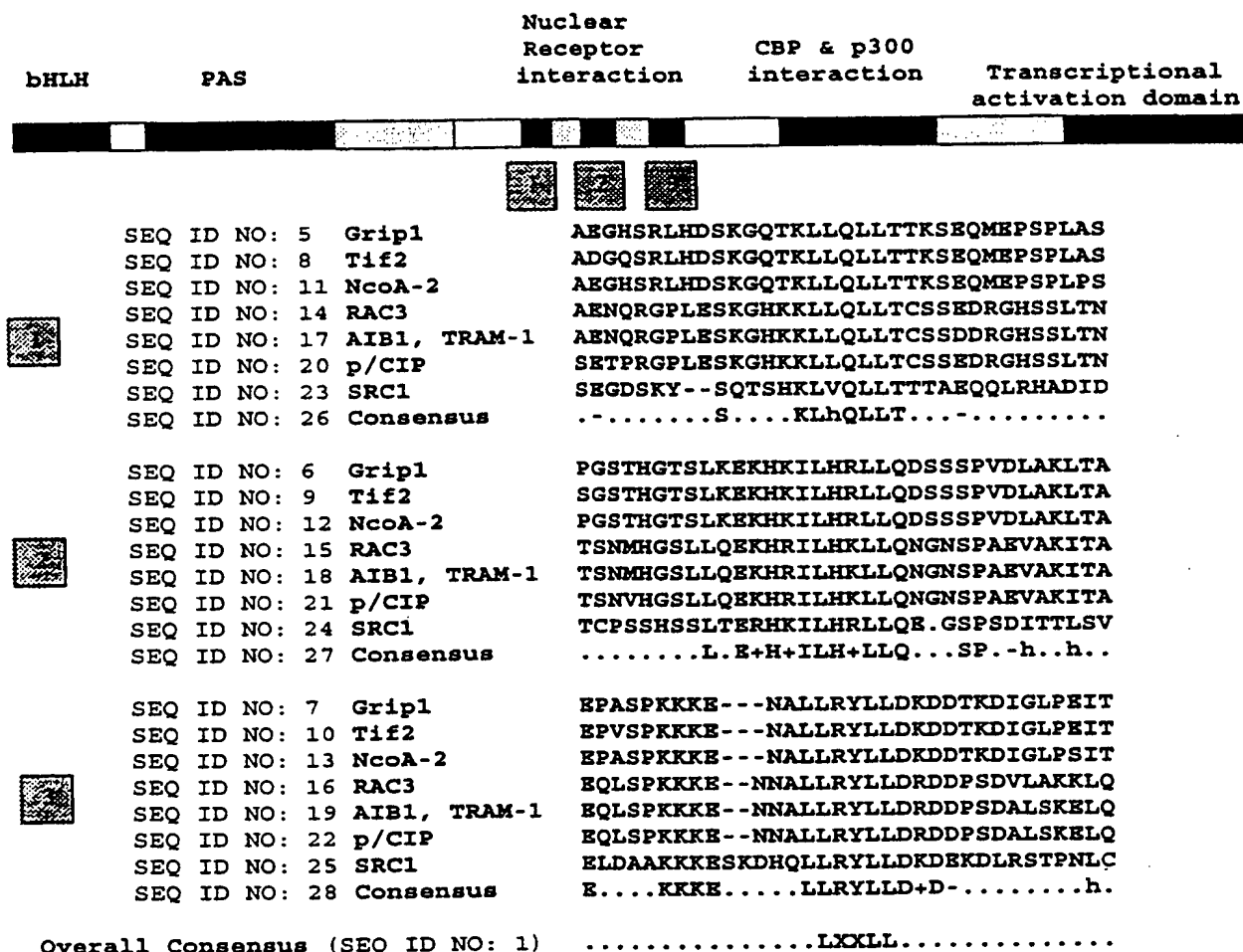


FIG. 5

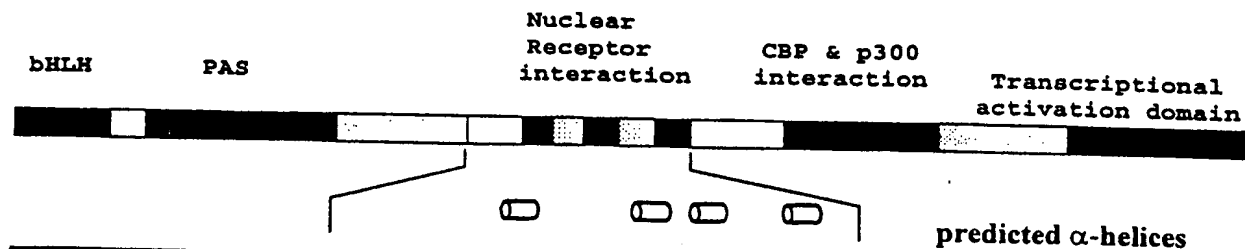
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FIGURE 6



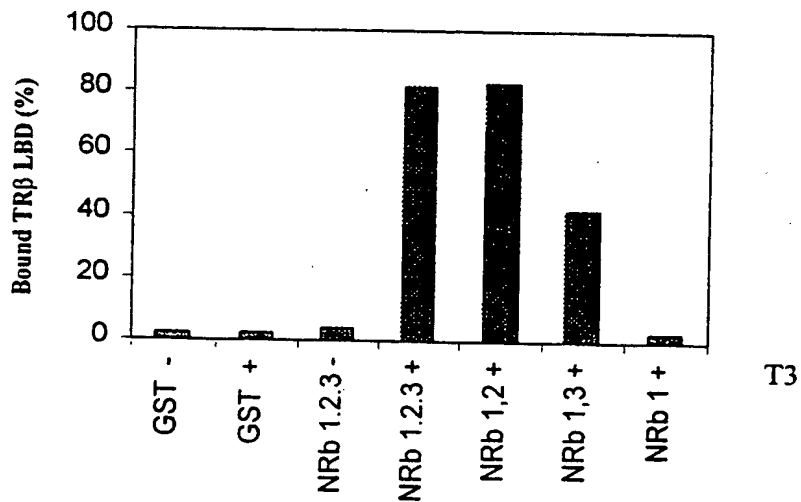
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FIGURE 7



GST

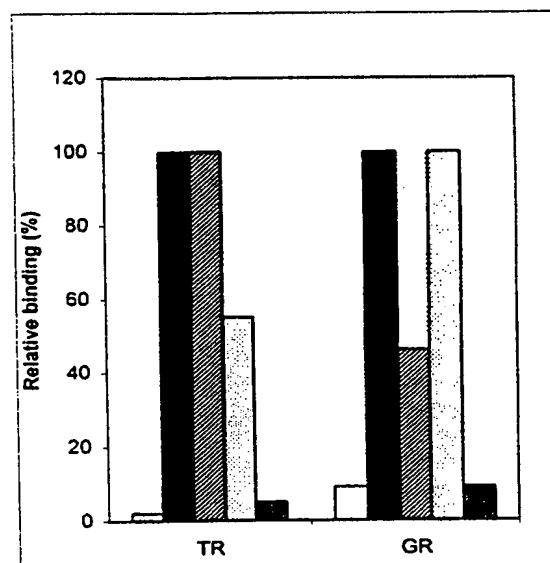
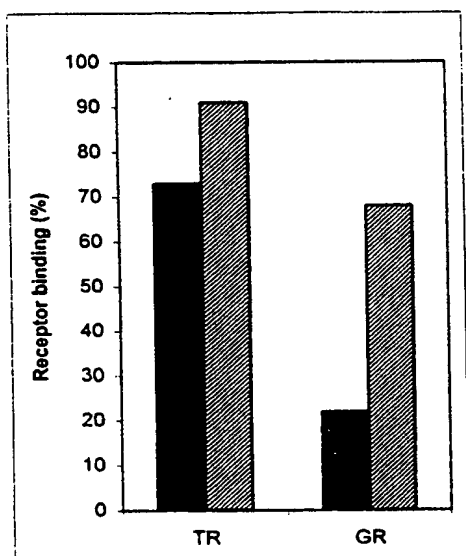
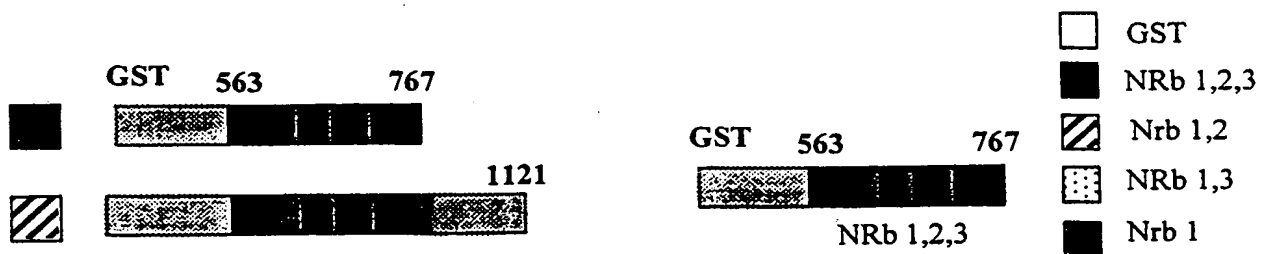
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| NRb 1,2 | KLLQLLT. | .ILHRLQ. | .AARAAAD |
| NRb 1,3 | KLLQLLT. | .AAHRAAQ. | .LLRYLLD |
| NRb 1 | KLLQLLT. | .AAHRAAQ. | .AARAAAD |



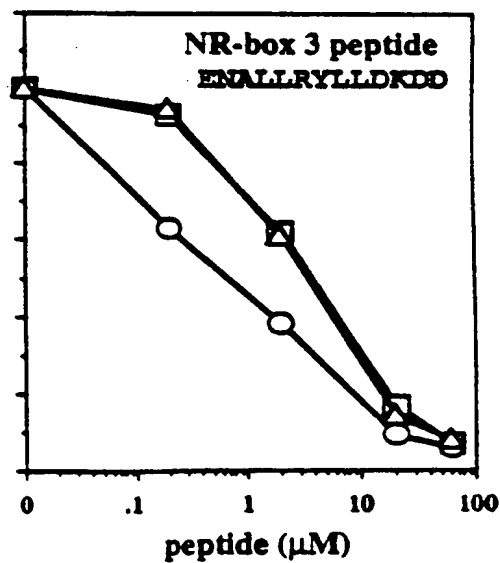
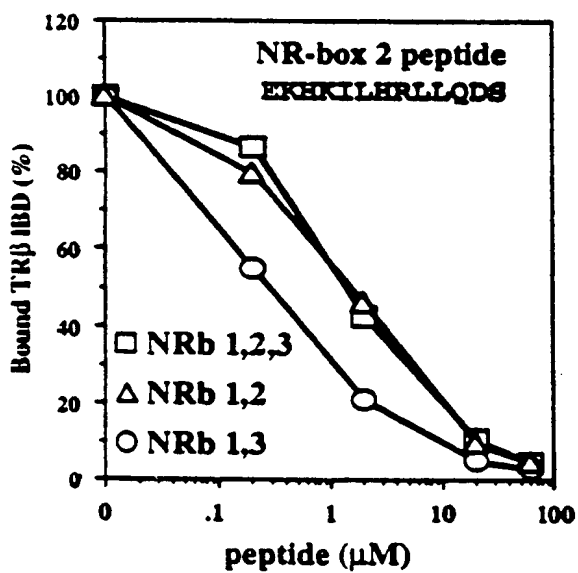
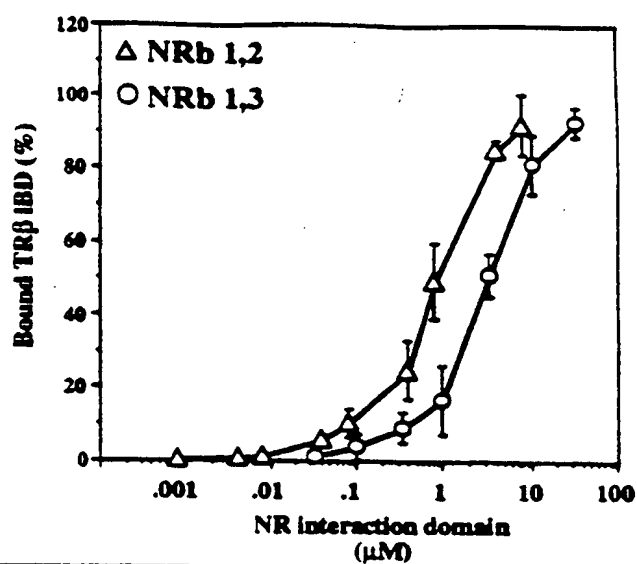
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FIGURE 8

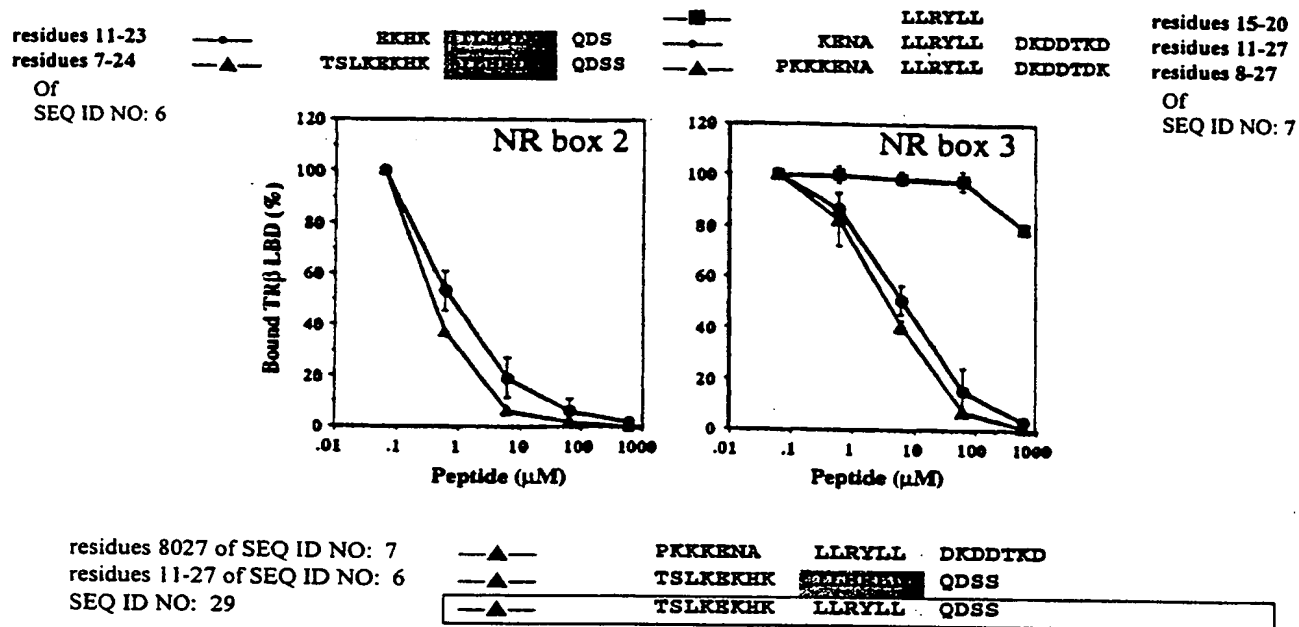


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FIGURE 9

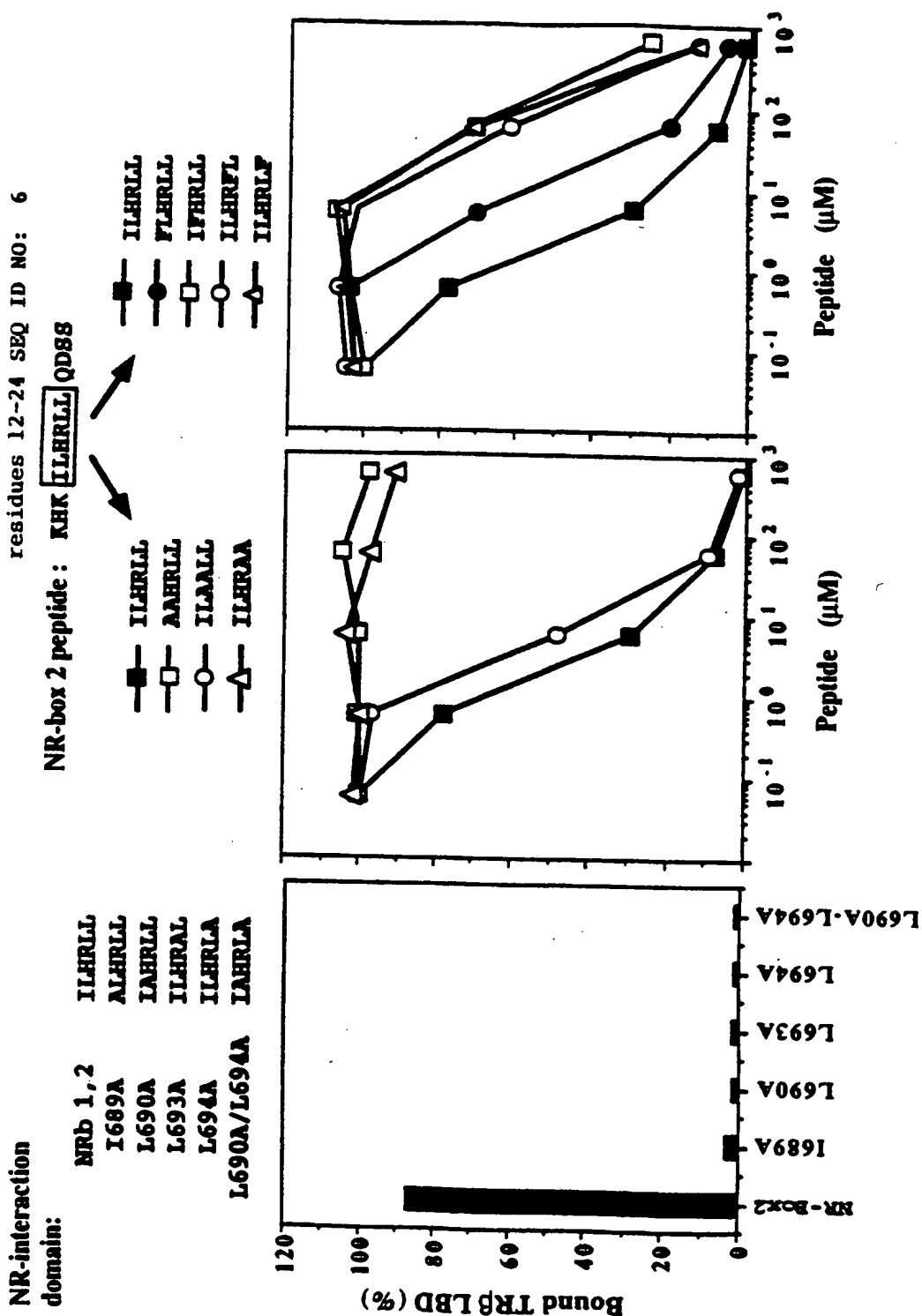
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FIGURE 10



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FIGURE 11



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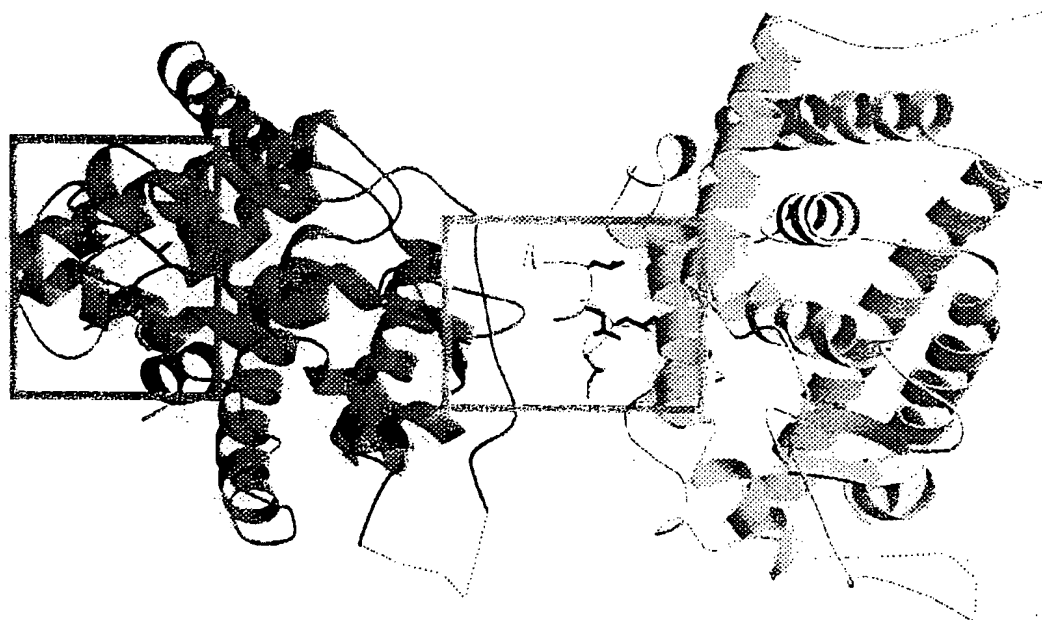


FIG. 12

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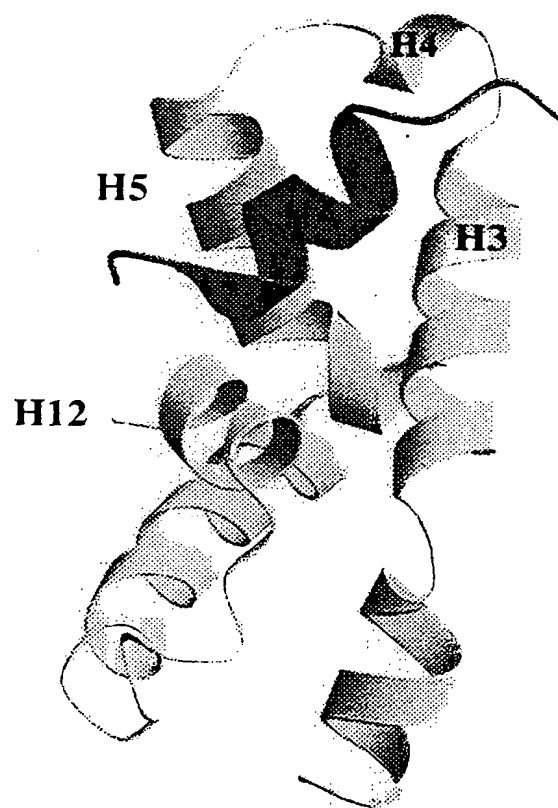
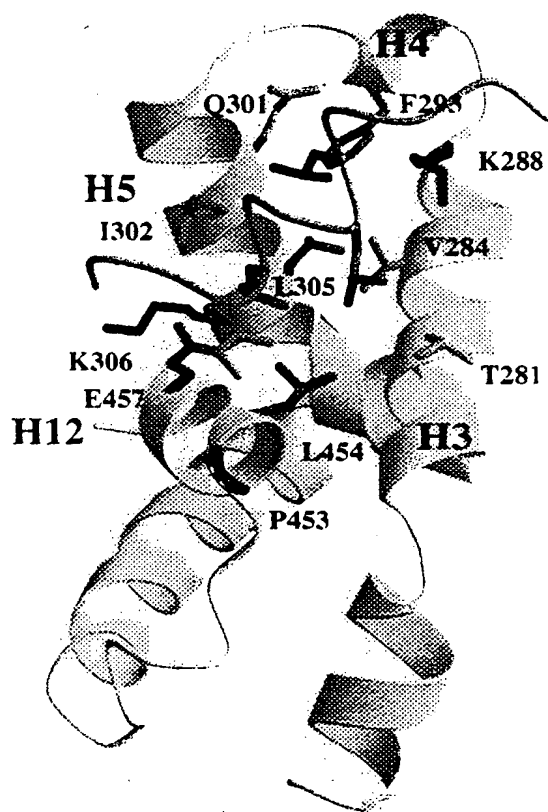


FIG. 13

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**FIG. 14**

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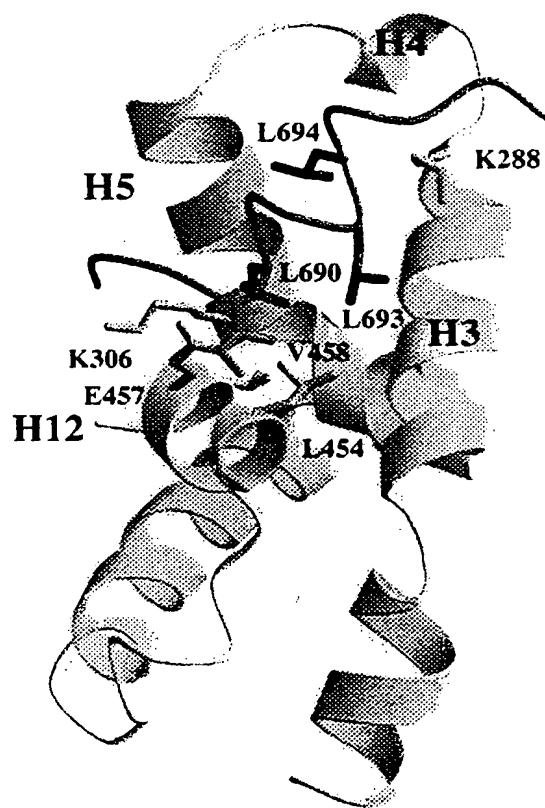


FIG. 15

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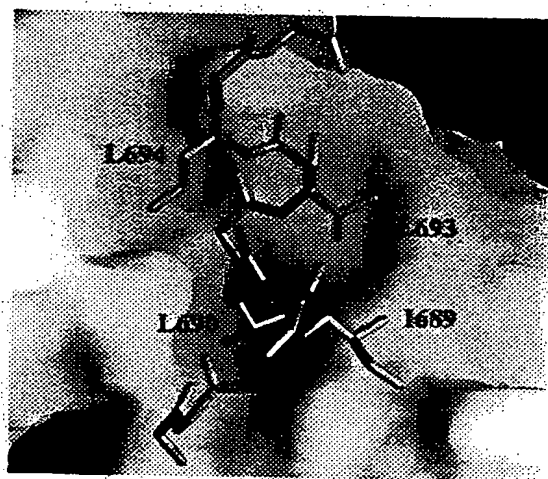


FIG. 16

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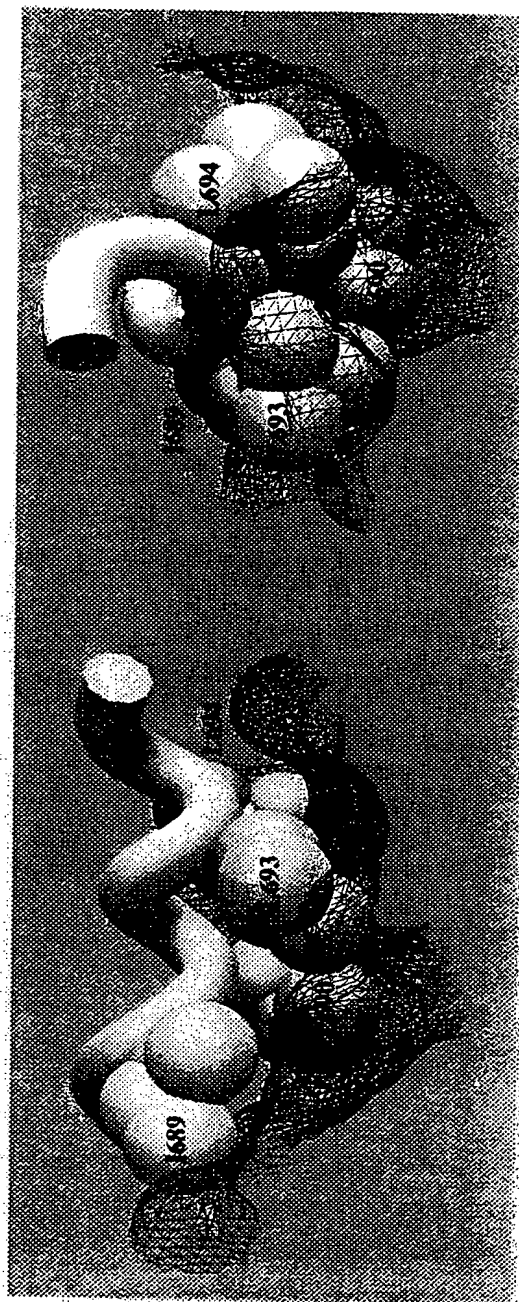


FIG. 17

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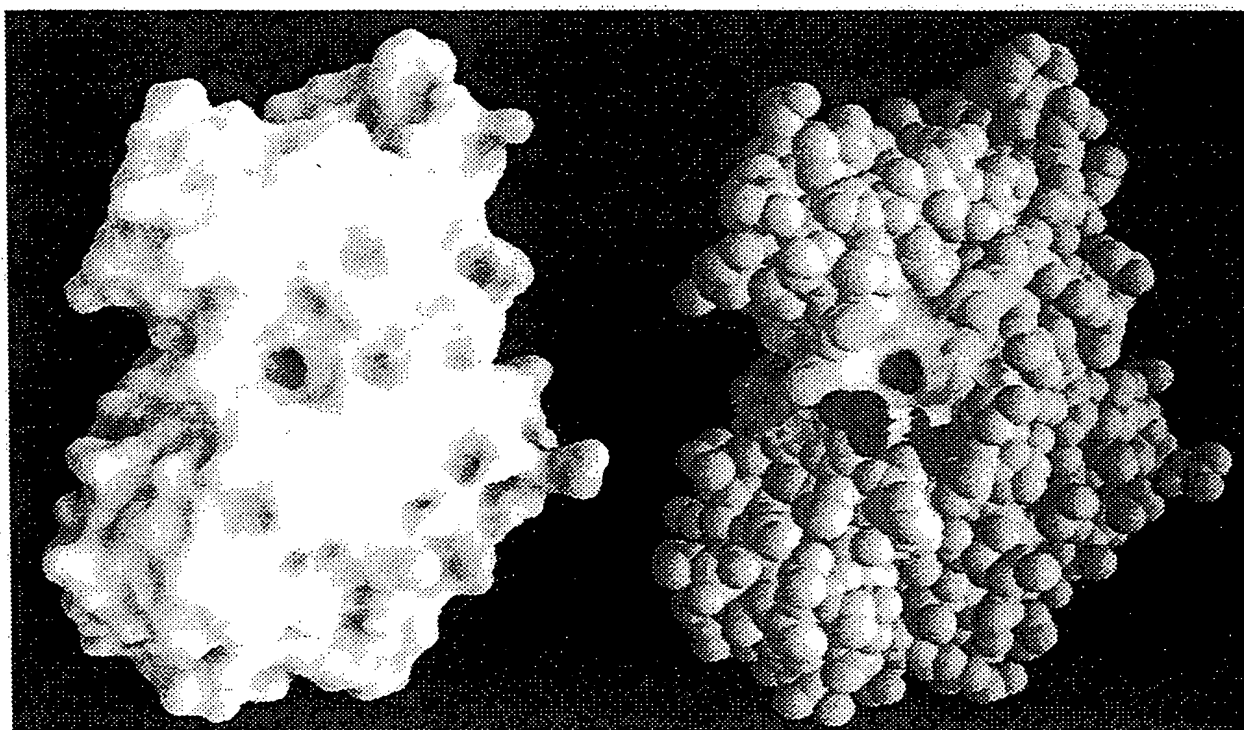


FIG. 18

5 SEQUENCE LISTING

10 <110> Baxter, John D.
Darimont, Beatrice
Feng, Weijun
Fletterick, Robert J.
Kushner, Peter J.
Wagner, Richard L.
West, Brian L.
Yamamoto, Keith R.

15 <120> METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR
COACTIVATOR BINDING

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Thr Ala

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<213> Homo sapiens

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 50 Val

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| (54) Title: METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR COACTIVATOR BINDING | | |
| (57) Abstract <p>The present invention relates to methods and agonist/antagonist compounds for modulating nuclear receptor coactivator binding. The invention includes a method for identifying residues comprising a coactivator binding site for a nuclear receptor of interest. Also included is a method of identifying agonists and/or antagonists that bind to a coactivator binding site of a nuclear receptor of interest. Agonists and antagonists of coactivator binding to nuclear receptors also are provided. The invention is exemplified by identification and manipulation of the coactivator binding site of the thyroid receptor (TR), and compounds that bind to these sites. The methods can be applied to other nuclear receptors including RAR, RXR, PPAR, VDR, ER, GR, PR, MR, and AR.</p> | | |

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INTERNATIONAL SEARCH REPORT

International application No.
PCT/US99/06899**A. CLASSIFICATION OF SUBJECT MATTER**

IPC(7) :G01N 33/50

US CL :435/7.1

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

U.S. : 435/7.1

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

Please See Extra Sheet.

C. DOCUMENTS CONSIDERED TO BE RELEVANT

| Category* | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No. |
|-----------------|---|-----------------------|
| X ----- A | WAGNER et al. A structural role for hormone in the thyroid hormone receptor. Nature. 14 December 1995, Vol. 378, pages 690-697, especially page 690 and figure 1 and 2 and Table 1. | 1 ----- 2-30 |

☐ Further documents are listed in the continuation of Box C. ☐ See patent family annex.

| | |
|---|--|
| * Special categories of cited documents: | *T* later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention |
| *A* document defining the general state of the art which is not considered to be of particular relevance | *X* document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone |
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| *O* document referring to an oral disclosure, use, exhibition or other means | |
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Date of the actual completion of the international search

01 DECEMBER 1999

Date of mailing of the international search report

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INTERNATIONAL SEARCH REPORT

International application No.

PCT/US99/06899

Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)

This international report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:

2. ☐ Claims Nos.:
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:

3. ☐ Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

Please See Extra Sheet.

1. ☒ As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.
2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. ☐ As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:

4. ☐ No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

☐

The additional search fees were accompanied by the applicant's protest.

☐

No protest accompanied the payment of additional search fees.

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(54) Title: METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR COACTIVATOR BINDING

(57) Abstract: The present invention relates to methods and agonist/antagonist compounds for modulating nuclear receptor coactivator binding. The invention includes a method for identifying residues comprising a coactivator binding site for a nuclear receptor of interest. Also included is a method of identifying agonists and/or antagonists that bind to a coactivator binding site of a nuclear receptor of interest. Agonists and antagonists of coactivator binding to nuclear receptors also are provided. The invention is exemplified by identification and manipulation of the coactivator binding site of the thyroid receptor (TR), and compounds that bind to these sites. The methods can be applied to other nuclear receptors including RAR, RXR, PPAR, VDR, ER, GR, PR, MR, and AR.

WO 99/060014 A3

METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR COACTIVATOR BINDING

ACKNOWLEDGEMENTS

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INTRODUCTION

Technical Field

The present invention relates to methods and compounds for modulating nuclear receptor coactivator binding.

Background

Cells contain receptors that can elicit a biological response by binding various molecules including proteins, hormones and/or drugs. Nuclear receptors represent a super family of proteins that are hormone/ligand-activated transcription factors that enhance or repress transcription in a cell type-, ligand- and promoter-dependent manner. The nuclear receptor family includes receptors for glucocorticoids (GRs), androgens (ARs), mineralocorticoids (MRs), progestins (PRs), estrogens (ERs), thyroid hormones (TRs), vitamin D (VDRs), retinoids (RARs and RXRs), peroxisomes (XPARs and PPARs) and icosanoids (IRs). The so-called "orphan receptors" for which ligands have not been identified are also part of the nuclear receptor superfamily, as they are structurally homologous to the classic nuclear receptors, such as steroid and thyroid receptors.

5 Although overall sequence conservation between nuclear receptors varies between different families
of receptors, sequence conservation between functional regions, or modules, of the receptors is
high. For example, nuclear receptors can be organized into functional modules comprising an N-
terminal transcriptional activation domain, a central DNA binding domain (DBD), and a C-terminal
10 ligand binding domain (LBD). The LBD of nuclear receptors represents a hormone/ligand-
dependent molecular switch. Binding of hormone to a nuclear receptor's LBD changes its ability to
modulate transcription of DNA, although they may have transcription-independent actions. Nuclear
receptors also bind proteins, such as chaperone complexes, corepressors, or coactivators, that are
involved in receptor function. Hormone binding by a nuclear receptor can increase or decrease
15 binding affinity to these proteins, and can influence or mediate the multiple actions of the nuclear
receptors on transcription. For example, nuclear receptors can stimulate transcription in response to
hormone binding by recruiting coactivator proteins to promoters of responsive genes (Glass et al.,
Curr. Opin. Cell Biol. (1997) 9:222-32); and Horwitz et al., *Mol. Endocrinol.* (1996) 10:1167-77).

Coactivators of the p160 family mediate activity of a transcriptional activation domain,
called AF2, that is part of the nuclear receptor's LBD. A few receptor mutants deficient in
20 coactivator-dependent activation have been isolated (TR: Collingwood et al. *Proc. Natl. Acad. Sci.*
(1997) 94:248-253; VDR: Jurutka et al., *J. Biol. Chem.* (1997) 272:14592-14599, Masayama et al.,
Mol. Endocrinol. (1997) 11:1507-1517; ER and RAR: Henttu et al., *Mol. Cell Biol.* (1997) 17:1832-
1839). While these studies support the physiological relevance of the observed interaction, the
structural and functional nature of the site to which coactivators bind has not been defined.

25 The medical importance of nuclear receptors is significant. They have been implicated in
breast cancer, prostate cancer, cardiac arrhythmia, infertility, osteoporosis, hyperthyroidism,
hypercholesterolemia, obesity and other conditions. However, limited treatments are available and
current agonist/antagonist drugs used to target nuclear receptors are ligands that bind to the
receptor's LBD buried deep within the receptor. Although additional targets on nuclear receptors
30 are desired for drug development, the structural and functional basis of such sites, including the
coactivator binding site, has not been described.

Accordingly, a need exists for identification and characterization of the coactivator binding
sites of nuclear receptors, and molecules that affect their interaction with cellular coactivator
proteins. This would provide a major new target for iterative drug design, synthesis, and selection.
35 It also would be advantageous to devise methods and compositions for reducing the time required to
discover compounds that target the coactivator binding site of nuclear receptors and administer
them to organisms to modulate physiological processes regulated by nuclear receptors.

5 **Relevant Literature**

Wagner et al., (*Nature* (1995) 378:690-697) disclose the crystal structure of rat TR-alpha LBD. Various references disclose mutations in carboxyl-terminal helices of nuclear receptors (Henttu et al., *supra*; O'Donnell et al., *Mol. Endocrinol.* (1991) 5:94-99; Whitfield et al., *Mol. Endocrinol.* (1995) 9:1166-79; Saatcioglu et al., *Mol. Cell Biol.* (1997) 17:4687-95; Collingwood et al., *supra*; Kamei et al., *Cell* (1996) 85:403-14). Hong et al. (*Proc. Natl. Acad. Sci. USA* (1996) 93(10):498-49452) and Hong et al. (*Mol. Cell. Biol.* (1997) 17:2735-2744) disclose cloning and expression of GRIP1 coactivator. Torchia et al., (*Nature* (1997) 387:677-84), Le Douarin et al., (*EMBO J* (1996) 15:6701-6715) and Heery et al. (*Nature* (1997) 387:733-736) disclose sequence alignment of various coactivator proteins showing a (SEQ ID NO: 1) LxxLL motif.

15

SUMMARY OF THE INVENTION

The present invention relates to identification and manipulation of the coactivator binding site of nuclear receptors. Identification of this site permits design and obtention of compounds that bind to the coactivator binding site of nuclear receptors and modulate coactivator binding to the receptor. The compounds include agonists and antagonists that modulate nuclear receptor activity by promoting (agonists) or blocking (antagonists) hormone-dependent coactivator binding to the receptor, particularly antagonists. The compounds of the invention can be receptor-, cell- and/or tissue-specific.

The present invention also includes protein cocrystals of nuclear receptors with a molecule bound to the coactivator binding site and methods for making them. The cocrystals provide means to obtain atomic modeling information of the specific amino acids and their atoms forming the coactivator binding site and that interact with molecules that bind to the site, such as coactivator. The cocrystals also provide modeling information regarding the coactivator:nuclear receptor interaction, as well as the structure of coactivators bound thereto.

The present invention further provides methods for identifying and designing small molecules that bind to the coactivator binding site using atomic models of nuclear receptors. The method involves modeling test compounds that fit spacially into a nuclear receptor coactivator binding site of interest using an atomic structural model comprising a nuclear receptor coactivator binding site or portion thereof, screening the test compounds in a biological assay characterized by

- 5 binding of a test compound to a nuclear receptor coactivator binding site, and identifying a test compound that modulates coactivator binding to the nuclear receptor.

The invention also includes compositions and methods for identifying coactivator binding sites of nuclear receptors. The methods involve examining the surface of a nuclear receptor of interest to identify residues that modulate coactivator binding. The residues can be identified by
10 homology to the coactivator binding site of human TR described herein. Overlays and superpositioning with a three dimensional model of a nuclear receptor LBD, or a portion thereof that contains a coactivator binding site, also can be used for this purpose. Additionally, alignment and/or modeling can be used as a guide for the placement of mutations on the LBD surface to characterize the nature of the site in the context of a cell.

- 15 Also provided is a method of modulating the activity of a nuclear receptor. The method can be *in vitro* or *in vivo*. The method comprises administering, *in vitro* or *in vivo*, a sufficient amount of a compound that binds to the coactivator binding site. Preferred compounds bind to the site with greater affinity than coactivator proteins found in a cell of interest. Binding at this site, the compound can compete for binding of coactivator proteins, thereby inhibiting gene transcription, or
20 in some cases promoting it, even when hormone is or is not bound.

The invention further includes a method for identifying an agonist or antagonist of coactivator binding to a nuclear receptor. The method comprises providing the atomic coordinates comprising a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system; modeling compounds which fit spacially into the nuclear receptor coactivator
25 binding site; and identifying in an assay for nuclear receptor activity a compound that increases or decreases activity of the nuclear receptor through binding the coactivator binding site.

Also provided is a machine-readable data storage medium with information for constructing and manipulating an atomic model comprising a coactivator binding site or portion thereof. The medium comprises a data storage material encoded with machine readable data which, when using a
30 machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex for a nuclear receptor coactivator binding site.

Also provided is a method of identifying a compound that selectively modulates the activity of one type of nuclear receptor compared to other nuclear receptors. The method is exemplified by
35 modeling test compounds that fit spacially and preferentially into a nuclear receptor coactivator

- 5 binding site of interest using an atomic structural model of a nuclear receptor coactivator binding site, selecting a compound that interacts with one or more residues of the coactivator binding site unique in the context of that site, and identifying in an assay for coactivator binding activity a compound that selectively binds to the coactivator binding site compared to other nuclear receptors. The unique features involved in receptor-selective coactivator binding can be identified by
10 comparing atomic models of different receptors or isoforms of the same type of receptor.

The invention finds use in the selection and characterization of peptide, peptidomimetic, as well as other small molecule compounds, such as small organic molecules, identified by the methods of the invention, particularly new lead compounds useful in treating nuclear receptor-based disorders.

15

BRIEF DESCRIPTION OF THE DRAWINGS

- Figure 1** shows the specific effects of mutations on hTR β 1 transcriptional activation in HeLa cells and correlation with effects on binding to GST-GRIP1. T₃ dependent activation of transcription of a reporter gene, expressed as the percentage of WT is plotted for each mutant.
20 GST-GRIP1 binding, analyzed by autoradiography after separation using 10% SDS-PAGE, was also expressed as the percentage of WT and plotted for each mutant. The GST-GRIP1 used included GRIP1 amino acids 721-1121; the same results were obtained using a GST-GRIP1 construct including GRIP1 amino acids 563-1121 (data not shown).

- Figure 2** shows that overexpression of full-length GRIP1 rescues loss of transcriptional
25 activation by hTR β 1 mutants. Indicated amounts of the expression vector for full-length GRIP1, pSG5-GRIP1, is included in the cotransfections, which otherwise are performed as in **Figure 1**. The WT or different representative hTR β 1 mutants are indicated.

- Figure 3** shows specific hER α surface mutants cause loss of transcriptional activation in HeLa cells in parallel with their loss of *in vitro* GRIP1 binding. The fold E₂ activation, expressed as
30 the percentage of WT, and the phosphorimager quantitation of *in vitro* binding of [³⁵S]-labeled hER α WT and mutants to GST-GRIP1 (GRIP1 amino acids 721-1121) also expressed as the percentage of WT is plotted for each mutant.

5 **Figure 4** shows a plot of the fold E_2 activation observed when the indicated amounts of the full-length GRIP1 expression vector, pSG5-GRIP1, are added to the co-transfection experiment, which otherwise is performed as for **Figure 3**. The WT or different hER α mutants are indicated. The data represent the averages of three independent experiments, with standard deviations less than 10%.

10 **Figure 5** shows a CPK model of the TR α -LBD, indicating the LBD surface locations of mutations made in the full-length hTR β 1. Mutated residues having no effect on GRIP1 binding or effect on activation in HeLa cells are shaded gray. Mutated residues with diminished GRIP1 and SRC-1 α binding and diminished activation in HeLa cells are colored to reflect chemical properties of the residues: red, blue (purple), and green indicate acidic, basic, and hydrophobic residues,
15 respectively. The main chain structures of the TR α - and TR β -LBDs are the same (data not shown).

Figure 6 shows sequence alignment of amino acid residues of members of the p160 coactivator family. Single amino acid designations are used. Members of the p160 coactivator family interact with the nuclear receptors through conserved (SEQ ID NO: 1) LxxLL motifs.

Figure 7 shows binding affinity assays of GST-GRIP1 constructs with NR-boxes 1, 2,
20 and/or 3 and their interaction with TR LBD. GRIP-1 NR boxes 1,2 and 3 interact differently with TR β LBD. Single letter designations are used for the amino acids.

Figure 8 shows binding affinity assays of GST-GRIP1 constructs with NR-boxes 1, 2, and/or 3 and their interaction with TR and GR LBDs. TR and GR differ in their interactions with GRIP-1.

25 **Figure 9** shows binding affinity assays for NR-box 2- and 3-peptides and GRIP1 and their interaction with TR LBD. NR box 2- and 3-containing peptides reproduce the affinity and specificity of the NR interaction domain.

Figure 10 shows binding affinity assays for NR-box 2- and 3-peptides and their interaction with TR LBD. Sequence adjacent to the (SEQ ID NO: 1) LxxLL motif modulate the affinity of
30 NR-box-TR β LBD interactions.

5 **Figure 11** shows binding affinity assays for mutant GRIP1 and NR-box 2- and 3-peptides and their interaction with TR LBD. The individual leucine residues of the (SEQ ID NO: 1) LxxLL motif are crucial for binding of the GRIP-1 NR interaction domain to TR β LBD.

10 **Figure 12** shows the contents of the asymmetric unit of the crystallized hTR β LBD:GRIP1 NR-box 2 peptide complex. The crystal lattice consists of a repeating unit containing a 2:2 complex of hTR LBD and GRIP1 site 2 peptide. Positions of the two GRIP1 site 2 peptides are boxed, in green (site1), and red (site 2), with the peptides drawn as a C-alpha trace. The two NCS related monomers of the hTR LBD are shown as a secondary structure ribbon drawing, with monomer 1 in light grey, and monomer 2 in dark grey. The side chains of the hydrophobic residues I689, L690, L693, L694 of the GRIP1 NR-box 2 peptides are drawn to emphasize those interactions observed in
15 both bound peptides.

Figure 13 shows a ribbon diagram depicting the interaction of the GRIP1 NR-box 2 peptide with the hTR β LBD. The GRIP1 NR-box 2 peptide (dark grey) forms three turns of α -helix, and binds the hTR LBD (light gray) in a hydrophobic cleft defined by helices H3, H4, H5, and H12. Portions of the hTR β LBD, and the neighboring monomer, are omitted for clarity.

20 **Figure 14** shows interface between the GRIP1 NR-box 2 peptide and the hTR β LBD. Side chains of residues of the hTR β LBD within 4.5Å of the GRIP-1 NR-box 2 peptide are labeled. The color of the individual side chains reflects the chemical nature of the residue: acidic residues are red, basic residue are blue, aliphatic residues are green, aromatic residues are brown, and polar residues are orange. The peptide is depicted as a C-alpha trace with the side chains of (SEQ ID
25 NO: 2) ILxxLL motif shown explicitly.

Figure 15 shows residues in the hTR β LBD that are necessary for transactivation. The transactivation mutations are mapped onto the interface between the GRIP1 NR-box 2 peptide and the hTR β LBD.

30 **Figure 16** shows molecular surface of the hTR LBD. The side chains of the leucines residues fit within a hydrophobic groove formed from helices H3, H5, and H12, while the side chain of the non-conserved isoleucine residue packs against the outside edge of the groove. The remainder of the peptide is shown as main chain.

5 **Figure 17** shows complementarity between the (SEQ ID NO: 1) LxxLL motif and the surface of the hTR LBD. The side chains of the (SEQ ID NO: 2) ILxxLL motif are shown in a CPK representation, with the main chain of the peptide drawn as a C-alpha trace. The three leucine residues fit into pockets of the coactivator binding site of the hTR β LBD, depicted as mesh, while the isoleucine residue rests on the edge of the site's cleft.

10 **Figure 18** shows the coactivator binding site cleft, one side of which is formed by conformationally hormone-responsive residues. On the left is a view of the TR-LBD molecular surface showing the concave surfaces in gray. The cavity is shown at the center of the figure. On the right is shown a CPK model of the TR-LBD, overlaid with a molecular surface view, which is restricted to a 12Å radius of the hydrophobic cavity. Mutated residues of the coactivator binding
15 site that are hormone-insensitive (V284, K288, I302 and K306) are located on one side of the cleft and are colored yellow. Mutated CBS residues likely undergo a conformational change upon hormone binding (L454 and E457) are located on the opposite side of the cleft and are colored red.

Figure 19 shows alignment of amino acid sequences (single letter amino acid designations) containing residues that form the coactivator binding sites of several nuclear receptors. The boxes
20 represent residues of alpha-helix (H3, H4, H5, H6 and H12); lower case letters "h" and "q" represent hydrophobic and polar residues, respectively.

5

DESCRIPTION OF SPECIFIC EMBODIMENTS

The present invention provides methods and compositions for identifying compounds that modulate nuclear receptor activity. The compounds can be nuclear receptor agonists or antagonists that bind to the coactivator binding site (and that act as mimetics to the coactivator in this regard), and promote (agonists) or block (antagonists) binding of the coactivator to the target nuclear receptor. Compounds that bind to the coactivator binding site also are provided. The compounds can be natural or synthetic. Preferred compounds are small organic molecules, peptides and peptidomimetics (e.g., cyclic peptides, peptide analogs, or constrained peptides).

As described in the Examples, mutagenesis and coactivator binding studies, coupled with analysis of atomic models derived from cocrystals, reveals for the first time a previously unknown structure for nuclear receptors, the coactivator binding site. By "coactivator binding site" is intended a structural segment or segments of nuclear receptor polypeptide chain folded in such a way so as to give the proper geometry and amino acid residue conformation for binding a coactivator. This is the physical arrangement of protein atoms in three-dimensional space forming a coactivator binding site pocket or cavity. Residues forming the site are amino acids corresponding to (i.e., the same as or equivalent to) human TR residues of C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Leu454, Glu457, Val458 and Phe459). The coactivator binding site is highly conserved among the nuclear receptor super family (Figure 19). Thus, this site corresponds to a surprisingly small cluster of residues on the surface of the LBD that form a prominent hydrophobic cleft. The hydrophobic cleft is formed by hydrophobic residues corresponding to human TR residues of C-terminal helix 3 (Ile280, Val283, Val284, and Ala287), helix 4 (Phe293), helix 5 (Ile302 and Leu305), helix 6 (Cys309), and helix 12 (Leu454, Val458 and Phe459). The hydrophobic cleft of the coactivator binding site also is highly conserved among the nuclear receptor super family (Figure 19).

The invention also includes compositions and methods for identifying coactivator binding sites of nuclear receptors. The methods involve examining the surface of a nuclear receptor of interest to identify residues that modulate coactivator binding. The residues can be identified by homology to the coactivator binding site of human TR described herein. A preferred method is alignment with the residues of any nuclear receptor corresponding to (i.e., equivalent to) human TR

5 residues of the C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459). Overlays and superpositioning with a three-dimensional model of a nuclear receptor LBD, or a portion thereof that contains a coactivator binding site, also can be used for this purpose. For example, three-dimensional structures of TR, RAR, RXR and ER
10 LBDs can be used for this purpose. For example, nuclear receptors identifiable by homology alignment include normal nuclear receptors or proteins structurally related to nuclear receptors found in humans, natural mutants of nuclear receptors found in humans, normal or mutant receptors found in animals, as well as non-mammalian organisms such as pests or infectious organisms, or viruses.

15 Alignment and/or modeling also can be used as a guide for the placement of mutations on the LBD surface to characterize the nature of the site in the context of a cell. Selected residues are mutated to preserve global receptor structure and solubility. To destroy the coactivator binding interaction, preferred mutations are to charged residues (e.g., Arg, Lys, or Glu) on the basis that bulky, surface charged residues might disrupt coactivator binding, yet preserve global receptor
20 structure and solubility. Mutants can be tested for coactivator binding as well as the relative change in strength of the binding interaction. Ligand-dependent coactivator interaction assays also can be tested for this purpose, such as those described herein.

Compounds that bind to the coactivator binding site of nuclear receptors can be identified by computational modeling and/or screening. For example, coactivator agonists or antagonists can be
25 identified by providing atomic coordinates comprising a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system, modeling them, and identifying compounds that fit spacially into the coactivator binding site. By a "portion thereof" is intended the atomic coordinates corresponding to a sufficient number of residues or their atoms of the coactivator binding site that interact with a compound capable of binding to the site. This includes receptor
30 residues having an atom within 4.5Å of a bound compound or fragment thereof. For instance, human TR residues V284, Phe293, Ile302, Leu305 and Leu454 contain side chain atoms that are within 4.5Å, and interact with, hydrophobic residues of a (SEQ ID NO: 1) LxxLL motif of an NR-box 2 coactivator peptide. As another example, an atomic structural model utilized for computational modeling and/or screening of compounds that bind to the coactivator binding site
35 may include a portion of atomic coordinates of amino acid residues corresponding to the site composed of residues of human thyroid receptor selected from Val284, Lys288, Ile302, Lys306, Leu454 and Glu457, or their structural and functional equivalents found in other receptors. Thus,

5 for example, the atomic coordinates provided to the modeling system can contain atoms of the nuclear receptor LBD, part of the LBD such as atoms corresponding to the coactivator binding site or a subset of atoms useful in the modeling and design of compounds that bind to a coactivator binding site.

10 The atomic coordinates of a compound that fits into the coactivator binding site also can be used for modeling to identify compounds or fragments that bind the site. By "modeling" is intended quantitative and qualitative analysis of molecular structure/function based on atomic structural information and receptor-coactivator agonists/antagonists interaction models. This includes conventional numeric-based molecular dynamic and energy minimization models, interactive computer graphic models, modified molecular mechanics models, distance geometry and
15 other structure-based constraint models. Modeling is preferably performed using a computer and may be further optimized using known methods. By "fits spacially" is intended that the three-dimensional structure of a compound is accommodated geometrically by a cavity or pocket of a nuclear receptor coactivator binding site.

20 Compounds of particular interest fit spacially and preferentially into the coactivator binding site. By "fits spacially and preferentially" is intended that a compound possesses a three-dimensional structure and conformation for selectively interacting with a nuclear receptor coactivator binding site. Compounds that fit spacially and preferentially into the coactivator binding site interact with amino acid residues forming the hydrophobic cleft of this site. In particular, the hydrophobic cleft of the coactivator binding site comprises a small cluster of
25 hydrophobic residues. The site also contains polar or charged residues at its periphery. The present invention also includes a method for identifying a compound capable of selectively modulating coactivator binding to different nuclear receptors. The method comprises the steps of modeling test compounds that fit spacially and preferentially into the coactivator binding site of a nuclear receptor of interest using an atomic structural model of a nuclear receptor, screening the test compounds in a
30 biological assay for nuclear receptor activity characterized by preferential binding of a test compound to the coactivator binding site of a nuclear receptor, and identifying a test compound that selectively modulates the activity of a nuclear receptor. Such receptor-specific compounds are selected that exploit differences between the coactivator binding sites of one type of receptor versus a second type of receptor, such as the differences depicted in Figure 19.

35 The invention also is applicable to generating new compounds that distinguish nuclear receptor isoforms. This can facilitate generation of either tissue-specific or function-specific compounds. For instance, GR subfamily members have usually one receptor encoded by a single

5 gene, although there are exceptions. For example, there are two PR isoforms, A and B, translated from the same mRNA by alternate initiation from different AUG codons. There are two GR forms, one of which does not bind ligand. This method is especially applicable to the TR subfamily which usually has several receptors that are encoded by at least two (TR: α , β) or three (RAR, RXR, and PPAR: α , β , γ) genes or have alternate RNA splicing.

10 The receptor-specific compounds of the invention preferably interact with conformationally constrained residues of the coactivator binding site that are conserved among one type of receptor compared to a second type of receptor. "Conformationally constrained" is intended to refer to the three-dimensional structure of a chemical or moiety thereof having certain rotations about its bonds fixed by various local geometric and physical-chemical constraints. Conformationally constrained
15 structural features of a coactivator binding site include residues that have their natural flexible conformations fixed by various geometric and physical-chemical constraints, such as local backbone, local side chain, and topological constraints. These types of constraints are exploited to restrict positioning of atoms involved in receptor-coactivator recognition and binding.

For instance, comparison of sequences of the GR and TR coactivator interaction surface
20 shows a highly negatively charged sequence at the C-terminal end of TR helix 12 (E460 and D461) that is neutral in the equivalent positions in GR helix 12 (GR residues T788 and N759, corresponding to TR residue positions 460 and 461, as depicted in **Figure 19**). As described in the Examples, the cocrystal of the hTR β LBD complexed with the GRIP1 NR-box 2 peptide shows that TR residues E460 and D461 interact with positively charged residues of the NR-box 2 peptide.
25 Also, when comparing the RAR LBD structure to that of the TR LBD, conformation of helix 12 differs slightly, whereas helices 3, 4, 5 and 6 are substantially the same. Thus, differences in helix 12, particularly charge differences at the C-terminal end of the helix, may modulate preferential interaction of TR for NR-box 2 containing coactivators. As further demonstrated in the Examples, TR and GR differ in their specificity for different NR-boxes containing the conserved (SEQ ID NO:
30 1) LxxLL motif found in members of the p160 family of coactivator proteins. As also demonstrated in the Examples, GR but not TR is able to interact with peptides containing the hydrophobic interaction motifs of p53 (SEQ ID NO: 3; FxxLW) and VP16 (SEQ ID NO: 4; FxxAL). Thus, TR exhibits preferential interaction with NR-box peptides comprising the (SEQ ID NO: 1) LxxLL motif, but GR does not discriminate and can bind peptides containing a generic amphipathic helix
35 motif. Accordingly, these real differences among the various nuclear receptors can be exploited in the identification and design of compounds that modulate coactivator binding to one nuclear receptor compared to another.

5 For modeling, docking algorithms and computer programs that employ them can be used to identify compounds that fit into the coactivator binding site. For example, docking programs can be used to predict how a small molecule of interest can interact with the nuclear receptor coactivator binding site. Fragment-based docking also can be used in building molecules *de novo* inside the coactivator binding site, by placing chemical fragments that complement the site to optimize
10 intermolecular interactions. The techniques can be used to optimize the geometry of the binding interactions. This design approach has been made possible by identification of the coactivator binding site structure thus, the principles of molecular recognition can now be used to design a compound which is complementary to the structure of this site. Compounds fitting the coactivator binding site serve as a starting point for an iterative design, synthesis and test cycle in which new
15 compounds are selected and optimized for desired properties including affinity, efficacy, and selectivity. For example, the compounds can be subjected to addition modification, such as replacement and/or addition of R-group substituents of a core structure identified for a particular class of binding compounds, modeling and/or activity screening if desired, and then subjected to additional rounds of testing.

20 Computationally small molecule databases can be screened for chemical entities or compounds that can bind in whole, or in part, to a nuclear receptor coactivator binding site of interest. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity (DesJalais et al., *J. Med. Chem.* (1988) 31:722-729) or by estimated interaction energy (Meng et al., *J. Comp. Chem.* (1992) 13:505-524). The molecule
25 databases include any virtual or physical database, such as electronic and physical compound library databases, and are preferably used in developing compounds that modulate coactivator binding.

Compounds can be designed intelligently by exploiting available structural and functional information by gaining an understanding of the quantitative structure-activity relationship (QSAR),
30 using that understanding to design new compound libraries, particularly focused libraries having chemical diversity of one or more particular groups of a core structure, and incorporating any structural data into that iterative design process. For example, one skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with the coactivator binding site of a nuclear receptor of interest. This process may begin by visual
35 inspection of, for example, the coactivator binding site on the computer screen. Selected fragments or chemical entities may then be positioned into all or part of the site. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and

- 5 molecular dynamics with standard molecular mechanics force-fields, such as CHARMM and AMBER.

For example, compounds and/or fragments can be designed to fill up the hydrophobic cleft, the pocket deep within the cleft, the upper end of the site, and/or the lower end of the site. Residues comprising a coactivator binding site, when defined by the user as those residues having an atom
10 within 4.5Å of an atom of a bound chemical entity, can be modeled to look for energetic contributions and interaction with the bound chemical entity. For example, a compound or fragment can be designed to contain hydrophobic groups that interact with hydrophobic residues of the coactivator binding site. As described in the examples, human TR residues V284, Phe293, Ile302, Leu305 and Leu454 contain side chain atoms that are within 4.5Å, and interact with,
15 hydrophobic residues of a (SEQ ID NO: 1) LxxLL motif of an NR-box 2 coactivator peptide. Thus, for example, peptides and/or peptide mimetics having a hxxhh motif, where "h" is a hydrophobic residue and x is any residue, can be constructed. Small organic molecules that mimic one or more of these particular interactions also can be designed, for example, by including one or more R-groups that are hydrophobic and fit into the site.

- 20 Specialized computer programs may also assist in the process of selecting chemical entity fragments or whole compounds. These include: GRID (Goodford, *J. Med. Chem.* (1985) 28:849-857; available from Oxford University, Oxford, UK); MCSS (Miranker et al., *Proteins: Structure, Function and Genetics*, (1991) 11:29-34; available from Molecular Simulations, Burlington, MA); AUTODOCK (Goodsell et al., *Proteins: Structure, Function and Genetics* (1990) 8:195-202;
25 available from Scripps Research Institute, La Jolla, CA); and DOCK (Kuntz et al, *J. Mol. Biol.* (1982) 161:269-288; available from University of California, San Francisco, CA).

Additional commercially available computer databases for small molecular compounds include Cambridge Structural Database and Fine Chemical Database (Rusinko, *Chem. Des. Auto. News* (1993) 8:44-47).

- 30 Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound. Assembly may be proceeded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of a nuclear receptor. This can be followed by manual model building using software such as Quanta or Sybyl.

5 Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include: CAVEAT (Bartlett et al., "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", In: *Molecular Recognition in Chemical and Biological Problems*", Special Pub., Royal Chem. Soc. (1989) 78:182-196; CAVEAT is available from the University of California, Berkeley, CA); 3D Database systems such as MACCS-3D (MDL
10 Information Systems, San Leandro, CA; reviewed in Martin, *J. Med. Chem.* (1992) 35:2145-2154); and HOOK (available from Molecular Simulations, Burlington, MA).

In addition to building a compound in a step-wise fashion, one fragment or chemical entity at a time as described above, compounds that bind to a coactivator binding site of interest also may be designed as a whole or *de novo* using either an empty coactivator binding site or optionally
15 including some portion(s) of a molecule known to binds to the site, such as an NR-box type peptide. These methods include: LUDI (Bohm, *J. Comp. Aid. Molec. Design* (1992) 6:61-78; LUDI is available from Biosym Technologies, San Diego, CA); LEGEND (Nishibata et al., *Tetrahedron* (1991) 47:8985; LEGEND is available from Molecular Simulations, Burlington, MA); and LeapFrog (available from Tripos Associates, St. Louis, MO).

20 Other molecular modeling techniques may also be employed in accordance with this invention. See, for example, Cohen et al., *J. Med. Chem.* (1990) 33:883-894); Navia et al., *Curr. Opin. Struct. Biol.* (1992) 2:202-210). For example, where the structures of test compounds are known, a model of the test compound may be superimposed over the model of the structure of the invention. Numerous methods and techniques are known in the art for performing this step, any of
25 which may be used. See, for example, Farmer, "Drug Design," Ariens, E.J., ed., 10:119-143 (Academic Press, New York, 1980); U.S. Patent No. 5,331,573; U.S. Patent No. 5,500,807; Verlinde, *Structure*, (1994) 2:577-587); and Kuntz et al., *Science*, (1992) 257:1078-1082). The model building techniques and computer evaluation systems described herein are not a limitation on the present invention.

30 Using these computer modeling systems a large number of compounds may be quickly and easily examined and expensive and lengthy biochemical testing avoided. Moreover, the need for actual synthesis of many compounds can be substantially reduced and/or effectively eliminated.

Compounds identified through modeling can be screened in an assay characterized by binding of the compound to a coactivator binding site of interest for coactivator binding activity,
35 such as a biologically based assay. Screening can be *in vitro* and/or *in vivo*. Preferred assays include cell-free competition assays and cell culture based assays. The biological screening

5 preferably centers on activity-based response models, binding assays (which measure how well a compound binds to the receptor), and bacterial, yeast and animal cell lines (which measure the biological effect of a compound in a cell). The assays can be automated for high capacity - high throughput screening (HTS) in which large numbers of compounds can be tested to identify compounds with the desired activity.

10 As an example, *in vitro* binding assays can be performed in which compounds are tested for their ability to block the binding of a coactivator protein, fragment, fusion or peptide thereof, to a coactivator binding site of interest. For cell and tissue culture assays, they may be performed to assess a compound's ability to block function of cellular coactivators, such as members of the p160 family of coactivator proteins, such as SRC-1, AIB1, RAC3, p/CIP, and GRIP1 and its homologues
15 TIF 2 and NcoA-2, and those that exhibit receptor and/or isoform-specific binding affinity. In a preferred embodiment, compounds of the invention bind to a nuclear receptor coactivator binding site with greater affinity than the cellular coactivator proteins. Tissue profiling and appropriate animal models also can be used to select compounds. Different cell types and tissues also can be used for these biological screening assays. Suitable assays for such screening are described herein
20 and in Shibata et al. (*Recent Prog. Horm. Res.* 52:141-164 (1997)); Tagami et al. (*Mol. Cell Biol.* (1997) 17(5):2642-2648); Zhu et al. (*J. Biol. Chem.* (1997) 272(14):9048-9054); Lin et al. (*Mol. Cell Biol.* (1997) 17(10):6131-6138); Kakizawa et al. (*J. Biol. Chem.* (1997) 272(38):23799-23804); and Chang et al. (*Proc. Natl. Acad. Sci. USA* (1997) 94(17):9040-9045), which references are incorporated herein in their entirety by reference. For example, coactivators or binding fragments
25 thereof can be expressed and/or assayed for binding as for GRIP1 (Hong et al., *MCB supra*; and Hong et al., *PNAS supra*) and/or SRC-1 (Spencer et al., *Nature* (1997) 389:194-198; Onate et al., *Science* (1995) 270:1354-1357), incorporated by reference.

The compounds selected can have agonist and/or antagonistic properties. The compounds also include those that exhibit new properties with varying mixtures of agonist and antagonist
30 activities, depending on the effects of altering coactivator binding in the context of different activities of nuclear receptors, either hormone-dependent or hormone-independent, which are mediated by proteins other than coactivators, and which interact with the receptors at locations other than the coactivator binding site. The compounds also include those, which through their binding to receptor locations that are conformationally sensitive to hormone binding, have allosteric
35 effects on the receptor by stabilizing or destabilizing the hormone-bound conformation of the receptor, or by directly inducing the same, similar, or different conformational changes induced in the receptor by the binding of hormone.

5 Of particular interest is use of such compounds in a method of modulating nuclear receptor activity in a mammal by administering to a mammal in need thereof a sufficient amount of a compound that fits spatially and preferentially into a coactivator binding site of a nuclear receptor of interest. By "modulating" is intended increasing or decreasing activity of a nuclear receptor. For example, pre-clinical candidate compounds can be tested in appropriate animal models in order to
10 measure efficacy, absorption, pharmacokinetics and toxicity following standard techniques known in the art. Compounds exhibiting desired properties are then tested in clinical trials for use in treatment of various nuclear receptor-based disorders. These include ER-based disorders, such as postmenopausal symptoms and cancer resulting from loss of estrogen production, and osteoporosis and cardiovascular disease stemming from traditional estrogen replacement therapy. Others include
15 TR-based disorders including cardiovascular disease, metabolic disorders, hyperthyroidism, glaucoma and skin disorders. GR-based disorders include Type II diabetes and inflammatory conditions such as rheumatic diseases.

 The invention also provides for cocrystals made from nuclear receptor ligand binding domains with a molecule bound to the coactivator binding site. As exemplified in the Examples,
20 TR LBDs are co-crystallized with a peptide molecule comprising a coactivator NR-box 2 peptide sequence bound to the coactivator binding site, and the hormone/ligand T₃.

 Crystals are made from purified nuclear receptor LBDs that are usually expressed by a cell culture, such as *E. coli*. Preferably, different crystals (cocrystals) for the same nuclear receptor are separately made using different coactivators-type molecules, such as protein fragments, fusions or
25 small peptides. The coactivator-type molecules preferably contain NR-box sequences necessary for binding to the coactivator binding site, or derivatives of NR-box sequences. Other molecules can be used in co-crystallization, such as small organics that bind to the coactivator or hormone binding site(s). Heavy atom substitutions can be included in the LBD and/or a co-crystallizing molecule.

 After the three dimensional structure of the cocrystal is determined, the structural
30 information can be used in computational methods to design synthetic compounds for the nuclear receptor, and further structure-activity relationships can be determined through routine testing using the assays described herein and known in the art.

 Since nuclear receptor LBDs may crystallize in more than one crystal form, the structure coordinates of such receptors or portions thereof, as provided in **Appendix 1**, are particularly useful
35 for solving the structure of those other crystal forms of nuclear receptors. They may also be used to

- 5 solve the structure of mutants or co-complexes of nuclear receptors having sufficient structural similarity.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, may be determined using the structure coordinates of this invention as provided in **Appendix 1**. This method will provide an accurate structural form for the
10 unknown crystal more quickly and efficiently than attempting to determine such information *ab initio*.

Atomic coordinate information gleaned from the crystals of the invention can be stored. In a preferred embodiment, the information is provided in the form of a machine-readable data storage medium. This medium contains information for constructing and/or manipulating an atomic model
15 of a coactivator binding site or portion thereof. For example, the machine readable data for the coactivator binding site comprises structure coordinates of amino acids corresponding to human TR amino acids selected from C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459), or a homologue of the molecule or molecular
20 complex comprising the site. The homologues comprise a coactivator binding site that has a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å. A preferred molecule or complex represents a compound bound to the coactivator binding site.

The machine-readable data storage medium can be used for interactive drug design and molecular replacement studies. For example, a data storage material is encoded with a first set of
25 machine-readable data that can be combined with a second set of machine-readable data. For molecular replacement, the first set of data can comprise a Fourier transform of at least a portion of the structural coordinates of the nuclear receptor or portion thereof of interest, and the second data set comprises an X-ray diffraction pattern of the molecule or molecular complex of interest. Using a machine programmed with instructions for using the first and second data sets a portion or all of
30 the structure coordinates corresponding to the second data can be determined.

Protein for crystals and assays described herein can be produced using expression and purification techniques described herein and known in the art. For example, high level expression of nuclear receptor LBDs can be obtained in suitable expression hosts such as *E. coli*. Expression of LBDs in *E. coli*, for example, includes the TR LBD and other nuclear receptors, including
35 members of the steroid/thyroid receptor superfamily, such as the receptors ER, AR, MR, PR, RAR, RXR and VDR. Yeast and other eukaryotic expression systems can be used with nuclear receptors

5 that bind heat shock proteins as these nuclear receptors are generally more difficult to express in bacteria, with the exception of ER, which can be expressed in bacteria. Representative nuclear receptors or their ligand binding domains have been cloned and sequenced: human RAR- α , human RAR- γ , human RXR- α , human RXR- α , human PPAR- α , human PPAR- β , human PPAR- γ , human VDR, human ER (as described in Seielstad *et al.*, *Molecular Endocrinol.*, (1995) 9:647-658,
10 incorporated herein by reference), human GR, human PR, human MR, and human AR. The LBD for each of these receptors has been identified.

Coactivator proteins can be expressed using techniques known in the art, particularly members of the p160 family of coactivator proteins that have been cloned and/or expressed previously, such as SRC-1, AIB1, RAC3, p/CIP, and GRIP1 and its homologues TIF 2 and NcoA-2.
15 A preferred method for expression of coactivator protein is to express a fragment that retains transcriptional activation activity using the "yeast 2-hybrid" method as described by Hong *et al.* (*PNAS supra*; and *MCB supra*), for GRIP1 expression, which reference is herein incorporated by reference.

The proteins can be expressed alone, as fragments of the mature or full-length sequence, or
20 as fusions to heterologous sequences. For example, TR can be expressed without any portion of the DBD or amino-terminal domain. Portions of the DBD or amino-terminus can be included if further structural information with amino acids adjacent the LBD is desired. Generally, for the TR the LBD used for crystals will be less than 300 amino acids in length. Preferably, the TR LBD will be at least 150 amino acids in length, more preferably at least 200 amino acids in length, and most
25 preferably at least 250 amino acids in length. For example the LBD used for crystallization can comprise amino acids spanning from Met 122 to Val 410 of the rat TR- α or Glu 202 to Asp 461 of the human TR- β .

Typically the LBDs are purified to homogeneity for crystallization. Purity of LBDs can be measured with sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE), mass
30 spectrometry (MS) and hydrophobic high performance liquid chromatography (HPLC). The purified LBD for crystallization should be at least 97.5 % pure, preferably at least 99.0% pure, more preferably at least 99.5% pure.

Initially, purification of the unliganded receptor can be obtained by conventional techniques, such as hydrophobic interaction chromatography (HPLC), ion exchange chromatography (HPLC),
35 and heparin affinity chromatography.

5 To achieve higher purification for improved crystals of nuclear receptors, especially the TR subfamily and TR, the receptors can be ligand-shift-purified using a column that separates the receptor according to charge, such as an ion exchange or hydrophobic interaction column, and then bind the eluted receptor with a ligand, especially an agonist. The ligand induces a change in the receptor's surface charge such that when re-chromatographed on the same column, ligand-bound
10 receptor is separated from unliganded receptor. Usually saturating concentrations of ligand are used in the column and the protein can be preincubated with the ligand prior to passing it over the column. The structural studies detailed herein indicate the general applicability of this technique for obtaining super-pure nuclear receptor LBDs for crystallization.

Purification can also be accomplished by use of a purification handle or "tag," such as with
15 at least one histidine amino acid engineered to reside on the end of the protein, such as on the N-terminus, and then using a nickel or cobalt chelation column for purification. (Janknecht et al., *Proc. Natl. Acad. Sci. USA*, (1991) 88:8972-8976) incorporated by reference.

Typically purified LBD, such as TR LBD, is equilibrated at a saturating concentration of ligand at a temperature that preserves the integrity of the protein. Ligand equilibration can be
20 established between 2 and 37°C, although the receptor tends to be more stable in the 2-20°C range. Preferably crystals are made with the hanging drop methods detailed herein. Regulated temperature control is desirable to improve crystal stability and quality. Temperatures between 4 and 25°C are generally used and it is often preferable to test crystallization over a range of temperatures. The crystals are then subjected to vapor diffusion and bombarded with x-rays to obtain x-ray diffraction
25 pattern following standard procedures.

For co-crystallization with a peptide that binds to the coactivator binding site, various concentrations of peptides containing a sequence that binds to a coactivator binding site of a nuclear receptor of interest can be used in microcrystallization trials, and the appropriate peptides selected for further crystallization. Any number of techniques, including those assays described herein can
30 assay peptides for binding to the coactivator binding site of a nuclear receptor of interest. In a preferred embodiment, a NR-box 2 sequence-containing peptide is used for crystallization with TR LBD. A preferred peptide contains a NR-box (SEQ ID NO: 1) LxxLL motif, and suitable flanking sequences necessary for binding and forming complex with coactivator binding site of the nuclear receptor of interest, such as a TR LBD. The binding peptides are then tested in crystallization trials
35 at various concentrations and ratios of concentrations with a nuclear receptor of interest, for example, as described herein and in the Examples. For crystallization trials with TR LBD, the hanging drop vapor diffusion method is preferred. Conditions of pH, solvent and solute

5 components and concentrations and temperature can be adjusted, for instance, as described in the Examples. In the hanging drop method, to obtain suitable crystals for x-ray diffraction analysis, seeding of prepared drops with microcrystals of the complex can be used. Collection of structural information can be determined by molecular replacement using the structure of TR LBD determined herein or previously by Wagner et al., supra. The structure is refined following
10 standard techniques known in the art.

There are many uses and advantages provided by the present invention. For example, the methods and compositions described herein are useful for identifying peptides, peptidomimetics or small natural or synthetic organic molecules that modulate nuclear receptor activity. The compounds are useful in treating nuclear receptor-based disorders. Methods and compositions of
15 the invention also find use in characterizing structure/function relationships of natural and synthetic coactivator compounds.

The following examples illustrate various aspects of this invention. These examples do not limit the scope of this invention.

5

EXAMPLES

Example 1: Expression and purification of wild-type and mutant nuclear receptors and coactivators

A. Human TR β LBD

Human TR β LBD (His6-E202-D461) was expressed and purified as described (Shiau et al.,
10 *Gene* (1996) 179(2):205-10). Briefly, the protein was expressed from pET (e.g., pET3 and pET28)
in BL21DE3 at 14°C, induced at OD(600nm) 0.7 with 1mM IPTG and incubation was extended for
24 hours. Cells were harvested and lysed in 50mM sodium-phosphate buffer (pH 8.0), 0.3M NaCl,
10% glycerol, 25mM β -mercaptoethanol and 0.1mM PMSF as described above. The lysate was
15 cleared by ultracentrifugation (Ti45, 36000 rpm, 1h, 4°C), loaded on a Talon column equilibrated in
the sodium phosphate buffer described above, washed with 12mM imidazole and eluted with an
imidazole gradient (12 - 300 mM). TR β LBD containing fractions were loaded in 0.6M ammonium
sulfate on a TSK-phenyl hydrophobic interaction column and eluted with a reverse ammonium
sulfate gradient [0.6 – 0 M] in 50% glycerol and 10% acetonitrile. Fractions containing TR β LBD
20 were tested for hormone binding, pooled and incubated with a 3-fold molar excess of T₃ (Sigma).
The hydrophobic interaction run was repeated with liganded receptor under the same conditions.
Liganded receptor, which elutes earlier than unliganded receptor, was collected and buffer changed
to 20mM Hepes pH7.0, 3mM DTT and 0.1 μ M T₃ using NAP columns (Pharmacia). For
crystallization, the protein was concentrated by ultrafiltration (Millipore UFV2BGC10
concentrators) to a final concentration of 9mg/ml. The yield was about 9.5mg protein per liter
25 bacterial culture.

B. Human TR mutants

Thirty-seven thyroid receptor mutants were created by synthesizing double-stranded
oligonucleotides which encode the mutant sequence and which have ends allowing them to be
ligated as a cassette using pairs of the NsiI, PstI, SstI, AlwNI, ApoI, PfiMI, BstXI, BseRI, BsmFI,
30 PvuII, NspI, SmaI, PmlI, BglII and BsmI restriction sites of the hTR β 1 cDNA sequence, or the 3'
plasmid polylinker SalI, or BamHI restriction sites. The hTR β 1 sequences thus mutated were
subcloned into the pCMX vector encoding the full-length 461 amino acid hTR β 1 sequence. Some
of the mutations of the hTR β 1 in the CMX vector and all three mutations of the hER α in the pSG5-
ER-HEGO vector (Tora et al., *EMBO* (1989) 8:1981) were created using Quick Change Site-

- 5 Directed Mutagenesis Kits (Stratagene). The mutated sequences were verified by DNA sequencing using Sequenase Kits (Stratagene).

C. Human ER α LBD

The human ER α -LBD 297-554 was overexpressed as described previously (Seielstad, et al., *supra*) in BL21(DE3)pLysS cells transformed with a modified pET-23d-ERG vector that contained
10 the sequence Met-Asp-Pro fused to residues 297 to 554 of the hER α (provided by Paul Sigler of Yale University). Clarified bacterial lysates were adjusted to 3 M in urea and 0.7 M in NaCl and then applied to a 10-ml column of estradiol-Sepharose (Greene, et al., *Proc. Natl. Acad. Sci. USA* (1980) 77:5115-5119; Landel, et al., *Mol. Endocrinol.* (1994) 8:1407-1419; Landel, et al., *J. Steroid Biochem. Molec. Biol.* (1997) 63:59-73).

15 To carboxymethylate the solvent-accessible cysteines, the bound hER α -LBD was treated with 5 mM iodoacetic acid in 10 mM Tris, pH 8.1, 250 mM NaSCN (Hegy, et al., *Steroids* (1996) 61:367-373). Protein was eluted with 3 x 10⁻⁵ M ligand (either DES or OHT) in 30-100 ml of 50 mM Tris, 1 mM EDTA, 1 mM DTT and 250 mM NaSCN, pH 8.5. The yield of hER α -LBD was typically close to 100% (Seielstad, et al., *Biochemistry* (1995) 34:12605-12615). The affinity-
20 purified material was concentrated and exchanged into 20 mM Tris, 1 mM EDTA, 4 mM DTT, pH 8.1 by ultrafiltration. The protein was bound to a Resource Q column (Pharmacia) and then eluted with a linear gradient of 25-350 mM NaCl in 20 mM Tris, pH 8.1, 1 mM DTT. The hER α -LBD-ligand complexes eluted at 150-200 mM NaCl. Pooled fractions were concentrated by ultrafiltration and analyzed by SDS-PAGE, native PAGE, and electrospray ionization mass
25 spectrometry.

D. Human ER mutants

To test the importance of the NR box peptide/LBD interface observed in the crystal, a series of site-directed mutations were introduced into the ER α LBD. These mutations were designed either to simultaneously perturb the structural integrity and the nonpolar character of the floor of the
30 binding groove (Ile 358->Arg, Val 376->Arg and Leu 539->Arg) or to prevent the formation of the capping interactions (Lys 362->Ala and Glu 542->Lys). Fusions of glutathione-S-transferase (GST) to the wild-type and mutant LBDs were analyzed for their ability to bind ³⁵S-labeled GRIP1 in the absence of ligand or in the presence of DES or OHT.

5 ³⁵S-labeled GRIP1 was incubated with either immobilized GST, immobilized wild type GST-hER α LBD, or immobilized mutant GST-LBDs in the absence of ligand or in the presence of DES or OHT. The bound GRIP1 was quantitated after SDS-PAGE. I358R, mutant LBD containing a Ile->Arg substitution at residue 358; K362A, mutant LBD containing a Lys->Ala substitution at residue 362; V376R, mutant LBD containing a Val->Arg substitution at residue 376;
10 L539R, mutant LBD containing a Leu->Arg substitution at residue 539; E542K, mutant LBD containing a Glu->Lys substitution at residue 542.

In the absence of ligand or in the presence of OHT, fusions to the wild-type protein and all of the mutant LBDs showed no detectable binding to GRIP1. The Ile 358->Arg, Val 376->Arg and Leu 539->Arg mutants were all unable to interact with coactivator in the presence of agonist,
15 confirming the importance of the packing interactions observed in the crystal. Disruption of either the N- or C-terminal capping interaction also compromised GRIP1 binding in the presence of agonist. Only the wild-type GST-LBD was able to recognize the coactivator in the presence of DES.

E. Human ER LBD-GST Fusion Protein

20 A fusion between glutathione-S-transferase (GST) and amino acids 282-595 of hER α was constructed by subcloning the EcoRI fragment from pSG5 ER α -LBD (Lopez et al., submitted manuscript) into pGEX-3X (Pharmacia). The Ile 358-> Arg, Lys 362->Ala, and Leu 539->Arg mutations were introduced into the GST-LBD construct using the QuikChange Kit (Stratagene) according to the manufacturer's instructions. The Val 376->Arg and Glu 542->Lys mutations were
25 created in the GST-LBD construct by subcloning the BsmI/HindIII fragments of derivatives of pSG5-ER-HEGO (Tora, et al., *supra*) into which these mutations had already been introduced. All constructs were verified by automated sequencing (University of Chicago Cancer Research Center DNA Sequencing Facility).

F. Radiolabeled full-length receptors and coactivator proteins

30 Wild-type (WT) or mutant pCMV-hTR β 1 vector and the pSG5-GRIP1 and pCMX-SRC-1a vectors were used to produce radiolabeled full-length receptors and coactivator proteins using the TNT coupled Reticulocyte Lysate System (Promega) and [³⁵S]-Met (DuPont). GST-GRIP1 (amino acids 721-1221), GST-GRIP1 (amino acids 563-1121), GST-SRC-1a (amino acids 381-882), GST-hTR β 1 (full-length, WT or mutants, WT provided by C. Costa), and the GST-hRXR α (full-length

- 5 provided by. C. Costa), fusion proteins were produced in *E. coli* strain HB101 as per the manufacturer's protocol (Pharmacia Biotech).

G. Coactivator GRIP1 563-767 His6 GST fusion protein

- GRIP1 563-767 was cloned as a Bam HI-Xho I fragment derived from pGEX-2TK GRIP1 563-1121 into the corresponding sites of pGEX-4T1. A His6-tag was added by inserting a Xho I-Nae I fragment of pET23a into Xho I-Bsa AI sites of this pGEX-4T1 construct yielding pGEX GRIP1 563-767His6. Mutants of GRIP1 563-767 were generated by PCR or single stranded mutagenesis using oligonucleotides carrying the mutations and a pSG5 GRIP1 vector as template. The mutations were confirmed by sequence analysis and integrated into pGEX GRIP1 563-767His6 as NgoMI - Xho I fragments. The GRIP1 563-767 His6 GST fusion protein was expressed in HB101 at 37°C. Protein expression was induced with 1mM IPTG at an optical density (600 nm) of 0.7 and extended for 4 hours after induction. Cells were harvested by centrifugation, resuspended in sonication buffer (20mM TrisHCl pH 8.0, 0.1M NaCl, 10%glycerol, 0.1mM PMSF and protease inhibitors (Complete, EDTA free, Boehringer Mannheim)). The resuspended cells were freeze-thawed once, incubated on ice with 0.1mg/ml lysozyme for 20 minutes and lysed per sonication. The lysate was cleared by ultracentrifugation (Ti 45, 36000rpm, 1h 4°C), the supernatant filtered (Costar 0.2µm top filter) and loaded on a Talon column (Clontech). The column was washed with 10 column volumes of sonication buffer supplemented with 12mM imidazole and eluted with an imidazole gradient [12 - 100mM]. At this step the fusion proteins are about 95% pure. Imidazole was removed by gelfiltration on NAP columns (Pharmacia), and protein concentrations determined using the Biorad protein assay. Equal concentrations of the different derivatives of the fusion fragment were incubated with glutathione agarose (1h, 4°C) which was equilibrated in binding buffer (sonication buffer supplemented with 1mM DTT, 1mM EDTA and 0.01% NP-40). Beads were washed with at least 20 volumes of this buffer, diluted in binding buffer with 20% glycerol to 40%, frozen in aliquots and stored at -70°C.

30 **H. Coactivator GRIP1 563-767 His6**

- GRIP1 563-767 was cloned as a Bam HI - Xho I fragment derived from pGEX GRIP1 563-767His6 into corresponding cloning sites of pET23a yielding pETGRIP1 563-767His6. The fragment was expressed in BL21DE3. Expression, cell lysis and Talon purification was identical as described for GST GRIP1 563-767His6. The protein eluted from a Talon column in two fractions, one at 12mM and one between 40 and 70mM imidazole. In the earlier eluting fraction the fragment was associated with a 70 kDa protein which was removed by a MonoQ run in 50mM TrisHCl

- 5 pH7.5, 10% glycerol, 1mM EDTA, 1mM DTT, 0.1mM PMSF and protease inhibitors. GRIP1 563-767His6 eluted in the flow through and was concentrated by ultrafiltration. At this step the protein was more than 95% pure.

Example 2: Peptide synthesis

- 10 Coactivator peptides were obtained using standard techniques. All peptides were HPLC purified and analyzed by mass spectroscopy. Peptide concentrations were either determined spectroscopically using the tyrosine signal ($A_{276} = 1450 \text{ M}^{-1}\text{cm}^{-1}$) or by amino acid analysis following standard techniques.

Example 3: Binding assays with nuclear receptors and coactivators

A. GST-GRIP Pull-down Assays and Peptide Competition Assays

- 15 Binding experiments were performed by mixing glutathione beads containing 10 μg of GST fusion proteins (Coomassie Plus Protein Assay Reagent, Pierce) with 1-2 μl of the [^{35}S]-labeled wild-type or mutant hTR β 1 (25 fmoles, 4000 cpm of receptor), or coactivators in 150 μl of binding buffer (20 mM HEPES, 150 mM KCl, 25 mM MgCl_2 , 10% glycerol, 1 mM dithiothreitol, 0.2 mM phenylmethylsulfonyl fluoride, and protease inhibitors) containing 2 mg/ml BSA for 1.5 hrs in the
20 presence or absence of 1 μM T_3 . Beads were washed 3 times with 1 ml of binding buffer and the bound proteins were separated using 10% SDS-PAGE and visualized by autoradiography. Binding was quantitated by phosphorimaging using ImageQuant (Molecular Dynamics).

- For *in vitro* binding studies GR, TR and their derivatives were translated in the presence of [^{35}S]methionine using the TNT Coupled Reticulocyte System (Promega). Separate translations were
25 performed in the presence and absence of 10 μM dexamethasone or 1 μM RU486 for GR and 10 μM triiodothyronine for TR. Expression was quantified by phosphorimager analysis (BAS2000, Fuji). For all binding assays 50 μl of a 20% bead suspension containing either 1.6 or 4.0 μM bound purified GST GRIP1 fragment (either 568-767 or 563-1121) was incubated with 0.2 μl or 1.4 μl *in vitro* transcribed and translated TR or GR, respectively. Binding was performed in the binding
30 buffer described above supplemented with 20 $\mu\text{g}/\text{ml}$ BSA and appropriate hormone. The chosen GST GRIP1 fragment concentrations were sufficient to bind either 70 or 100% of the TR derivatives. The reaction was incubated at 4°C under rotation for 2 hours. In case of competition experiments, the appropriate concentration of peptides were added to the reaction before addition of

5 receptors. However, no differences in the results were noted by adding the peptides after half of the incubation of the GST GRIP1 fragment with nuclear receptors. This demonstrates that equilibrium is reached under the chosen conditions. Beads were washed five times with 200 μ l binding buffer + BSA at 4°C before elution of the bound proteins in 20 μ l SDS loading buffer. Eluted beads and input labeled protein were subjected to SDS-PAGE. The fraction of bound nuclear receptors was
10 determined by phosphoimager analysis.

B. GST-hTR β 1 Pull-down Assays

Assay and analysis was performed as for Example 3A. *In vitro* binding of [35 S]-labeled full-length GRIP1, [35 S]-labeled full-length SRC-1a, and [35 S]-labeled full-length hRXR α , to GST-hTR β 1 wild-type (WT) and mutants was performed. Mutants V284R, K288A, I302R, L454R, and
15 E457K all bound to hRXR α with an affinity equivalent to wild type hTR. All of these mutants showed decreased ability to bind GRIP1 and SRC-1a, as expected from the results of Example 3A. The same results were obtained when a GST-SRC1 construct including SRC-1a amino acids 381-882 was tested for binding of [35 S]-Met-labeled full-length hTR β 1 WT and mutants (data not shown).

20 C. GST-hER α LBD Pull-down Assays

The wild-type and mutant GST-hER α LBDs were expressed in BL21(DE3) cells. Total ligand binding activity was determined by a controlled pore glass bead assay (Greene, et al., *Mol. Endocrinol.* (1988) 2:714-726) and protein levels were monitored by western blotting with a monoclonal antibody to hER α (H222). Cleared extracts containing the GST- hER α LBDs were
25 incubated in buffer alone (50 mM Tris, pH 7.4, 150 mM NaCl, 2 mM EDTA, 1 mM DTT, 0.5% NP-40 and a protease inhibitor cocktail) or with 1 μ M of either DES or OHT for 1 hour at 4°C. Extract samples containing thirty pmol of GST-LBD were then incubated with 10 μ l glutathione-Sepharose-4B beads (Pharmacia) for 1 hour at 4°C. Beads were washed five times with 20 mM HEPES, pH 7.4, 400 mM NaCl, and 0.05% NP-40. 35 S-labeled GRIP1 was synthesized by *in vitro*
30 transcription and translation using the TNT Coupled Reticulocyte Lysate System (Promega) according to the manufacturer's instructions and pSG5-GRIP1 as the template. Immobilized GST-hER α LBDs were incubated for 2.5 hours with 2.5 μ l aliquots of crude translation reaction mixture diluted in 300 μ l of Tris-buffered saline (TBS). After five washes in TBS containing 0.05% NP-40,

- 5 proteins were eluted by boiling the beads for 10 minutes in sample buffer. Bound ^{35}S -GRIP1 was quantitated by fluorography following SDS-PAGE.

D. Electrophoretic Mobility Shift Assays

GRIP1, a mouse p160 coactivator, recognizes the ER α LBD in a ligand-dependent manner. The binding of agonists to the ER α LBD promotes recruitment of GRIP1, whereas binding of
10 antagonists prevents this interaction (Norris, et al., *J. Biol. Chem.* (1998) 273:6679-88). While agonist-bound receptor will bind to all three of the NR boxes from GRIP1, ER α strongly prefers NR-box 2 (Ding, et al., *Mol. Endocrinol.* (1998) 12:302-13).

An electrophoretic mobility shift assay was used to directly assess the ability of the NR-box 2 peptide to bind the purified ER α LBD in the presence of either DES or OHT. Eight microgram
15 samples of purified hER α -LBD bound to either DES or OHT were incubated in the absence of the peptide, i.e., buffer alone, or in the presence of either a 2-fold or 10-fold molar excess of the GRIP1 NR-box 2 peptide. The binding reactions were performed on ice for 45 minutes in 10 μl of buffer containing 20mM Tris, pH 8.1, 1mM DTT, and 200mM NaCl and then subjected to 6% native PAGE. Gels were stained with GELCODE Blue Stain reagent (Pierce).

20 In the presence of the NR-box 2 peptide, the migration of the DES-hER α -LBD complex was retarded. In contrast, peptide addition had no effect on the mobility of the OHT-hER α -LBD complex. Hence, this peptide fragment of GRIP1 possesses the ligand-dependent receptor binding activity characteristic of the full-length protein.

Example: 4 Transfection assays with TR and hER α

25 HeLa cell transfection and assay conditions are described (Webb et al., *Mol Endocrinol* (1995) 9:443). For TR assays, 5 μg of the reporter p(DR-4) $_2$ -TK-LUC consisting of two copies of the DR-4 element (a direct repeat of the consensus TR response element (TRE) spaced by 4 base pairs) placed upstream of a minimal (-32/+45) thymidine kinase gene promoter linked to luciferase (LUC) coding sequences were used. A reporter containing palindromic TREs gave the same results
30 (data not shown). Also, 2 μg of the hTR β 1 expression vector, pCMX-TR (WT or mutant), and 0.5 μg transfection control vector, pJ3LacZ, which contains the SV40 promoter linked to the β -galactosidase gene, were used. Other cells co-transfected with vector or receptor constructs can be used for same purpose. Alternative cells expressing sufficient levels of an endogenous receptor(s),

- 5 or cells selected that express a single reporter, can be used for transfection assays, including MCF-7 cells expressing ER (Webb et al., *supra*), and GC cells expressing TR (Norman et al., *J. Biol. Chem.* (1989) 264:12063-12073).

For hER α assays, 5 μ g of estrogen responsive reporter plasmid encoding chloramphenicol acetyltransferase (CAT), pERE-collTATA (Sadovsky, *et al.*, *Mol Cell Biol.* (1995) 15:1554), 0.5 μ g
 10 expression vector encoding full-length hER α , pSG5-er HEGO (WT or mutants), and 2 μ g of pj3lacZ, were used. For the experiments of Figures 2 and 4, 0.5 μ g of a full-length GRIP1 expression vector, pSG5-GRIP1, was also included in the transfection. Transfected cells were treated with or without 1 μ M T₃ or E₂, as indicated. After culturing for 24 hrs, the LUC or CAT activities were assayed and the β -galactosidase activities were also assayed to correct for
 15 differences in transfection efficiencies. The triplicate points were averaged and standard deviations were less than 10%.

Example 5: Hormone binding assays for wild-type and mutant TRs

The T₃ binding affinity constants (K_d) for *in vitro* -translated WT and mutant TRs were measured using [¹²⁵I] 3,5,3'-triiodo-L-thyronine ([¹²⁵I]T₃) in gel filtration binding assays as
 20 described (Apriletti et al., *Protein Expr. Purif.* (1995) 6:363). Both the K_d and standard error (S.E.) values were calculated using the Prism computer program (GraphPad Software, Inc.). Mutations are indicated by the single-letter amino acid abbreviations, with the native residue name, followed by the primary sequence position number, and then the mutated residue name. The affinity of the WT TR is 81 \pm 12 pM. The relative affinity was determined by dividing the WT K_d by each
 25 mutant K_d. The 37 mutants tested with their relative affinities are: E217R (123%), E227R (109%), K242E (92%), E267R (117%), H271R (123%), T277R (7%), T281R (145%), V284R (105%), D285A (89%), K288A (98%), C294K (94%), E295R (118%), C298A (87%), C298R (141%), E299A (171%), I302A (86%), I302R (99%), K306A (6%), K306E (6%), P384R (164%), A387R (107%), E390R (151%), E393R (146%), L400R (95%), H413R (109%), H416R (153%), M423R
 30 (156%), R429A (48%), S437R (170%), L440R (174%), V444R (89%), T448R (234%), E449R (36%), P453E (32%), L454R (26%), L456R (46%), E457K (71%).

Example 6: Coactivator binding assays for wild-type and mutant TRs

Wild type (WT) TR and most of the TR mutants liganded to 3,5,3'-triiodo-L-thyronine (T₃) bind equally well to the coactivator, GRIP1. In all cases, GRIP1 binding was hormone-dependent

5 (data not shown). Mutations L454R and E457K in surface residues of helix 12 abolish GRIP1 binding (**Figure 1**). Mutations in two residues of helix 3, V284R and K288A, and two residues of helix 5, I302R and K306A, also impair binding (**Figure 1**). Five mutations with diminished GRIP1 binding (V284R, K288A, I302R, L454R, and E457K) also show decreased binding to another coactivator, SRC-1a (data not shown). Thus, these results show that two different coactivators
10 recognize the same TR surface residues.

Example 7: TR residues involved in ligand-dependent transcription activation in context of a cell

Residues involved in ligand-mediated transcription activation were identified by testing the TR mutants of Example 8 in HeLa cells. T₃ increased reporter gene activity 5-fold in cells
15 expressing either WT TR or mutated TRs showing normal GRIP1 binding (representative mutants are shown in **Figure 1**). By contrast, TR mutants with diminished or absent GRIP1 binding (V284R, K288A, I302R, K306A, L454R, and E457K) show a diminished or absent response to T₃ which correlates with the GRIP1 binding defect. Overexpression of GRIP1 increases activation by the WT TR and rescues activation by TR mutants roughly in proportion to the severity of the defect of
20 GRIP1 binding and activation (**Figure 2**). These results suggest that the same residues are required for coactivator binding, function of the endogenous coactivator(s) in HeLa cells, and responsiveness of TRs to GRIP1.

Example 8: Effect of TR mutations on other receptor functions

The effects of the mutations on other receptor functions also were examined. All of the
25 mutants bound radiolabeled thyroid hormone (K_d values, 6%-234% that for native receptor); occasional lower values were expected because some residues have partially buried side chains. None of the residues that decrease GRIP1 binding affected TR binding to a GST-RXR fusion protein or to DNA using three different DNA half-site arrangements and testing with or without added RXR (data not shown). Some mutations that affect GRIP1 binding occur in a region
30 spanning helices 3-5, which has been suggested as important for TR/RXR heterodimerization (O'Donnell et al., *supra*; Lee et al., *Mol. Endocrinol.* (1992) 6:1867-1873). In contrast, however, the above results indicate that these residues do not contribute to TR/RXR heterodimerization. Further, TRs mutated in the CBS residues retain the ability of WT TR of T₃-dependent inhibition of the activity of the Jun and Fos transcription factors at an AP-1 site (Saatcioglu et al., *supra*), suggesting
35 that the CBS residues do not participate in TR actions mediated through these proteins. These data

- 5 indicate that the mutational effects are specific, the amount of input labeled TR in the different reactions is comparable, and the levels of expression of the mutant TRs are comparable to those of WT receptors.

Example 9: Coactivator binding site in ER

- Three separate mutations (K362A, V376R, and E542K) were created in human estrogen
10 receptor- α (hER α) which align to three of the effective positions in hTR β 1 (K288A, I302R, and E457K). All three mutations diminish GRIP1 binding and abolish transcriptional activation (Figure 3), and mutant V376R, with 10% residual GRIP1 binding, was rescued partially by overexpression of GRIP1 (Figure 4). As a control, the ER mutants demonstrated a normal hormone-dependent ability to activate a vitellogenin-LUC hybrid reporter gene, GL45, which
15 responds to the ER amino-terminal activation function (Berry et al., *EMBO J* (1990) 9:2811-2818) (data not shown). The finding that similar residues are required for GRIP1 binding and transcription activation activity in the TR and ER suggests that the coactivator binding site residues are similar in different nuclear receptors.

Example 10: Coactivator NR-box binding affinity for TR

- 20 To study the interaction between nuclear receptors and GRIP1 *in vitro*, a fragment of GRIP1 (563-767) was purified that contains all three NR-boxes (Figures 6 and 7). The fragment was found to be highly soluble and, in agreement with a secondary structure prediction using PhD, displays a mainly alpha-helical far UV-CD spectrum (data not shown). Three of the four helices predicted for the fragment include the NR-boxes at their C-terminus, suggesting that these boxes are
25 part of amphipathic alpha-helices. These results show that the NR-boxes of GRIP1 are contained in a soluble, alpha-helical 24kD fragment.

- Binding assays show that GRIP1 NR-boxes 1, 2 and 3, interact differentially with hTR β LBD (Figure 7). A GST-fusion of the GRIP1 (563-767) fragment strongly binds TR (kD or EC50) in a ligand depend fashion. Replacement of the hydrophobic residues of NR-box 3 with alanine
30 does not reduce binding of TR significantly, whereas similar replacement of NR-box 2 results in loss of TR binding of about 50%. By titrating the amount of GRIP1 fragment, about a 4-fold stronger binding of TR for NR-box 2 (EC50 = 1.0 μ M) over NR-box 3 (EC50 = 4.0 μ M) was estimated. In the absence of functional NR-boxes 2 and 3, almost no binding to TR was detected suggesting that under these experimental conditions NR-box 1 is not a cognate binding site for TR.

- 5 Full length TR or TR-LBD bound GRIP1 equally. These results show that TR recognizes GRIP1 NR-box 2 and 3, with preference for NR-box 2.

Example 11: Coactivator NR-box binding affinity for GR

GR also was found to bind GRIP1 (563-767) in a ligand-dependent manner (Figure 8). However, in contrast to TR, extension of GRIP1 (563-767) to residue 1121 increases binding to GR about 3-fold suggesting an additional binding site on GRIP1 for GR. Binding of the larger fragment remains ligand-dependent; no interaction can be observed in the presence of the GR partial antagonist RU486. These results are in agreement with *in vivo* 2-hybrid GR GRIP1 interaction studies. In the presence of ligand no difference was detected in the binding of GRIP1 by full length GR or a deletion mutant of GR that lacks the N-terminal activation domain AF-1. However in the absence of ligand, binding of GR to GRIP1 (563-1121) increased by about 10-fold indicating that sequences in the GR N-terminus are able to suppress binding of unliganded GR to this additional binding site in GRIP1. Additionally, GR did not bind to a GRIP1 (563-767) mutant in which both NR-box 2 and 3 are replaced by alanines, and binds most strongly to a fragment that lacks a functional NR-box 2. As with TR, GR does not recognize NR-box 1. In contrast to TR, the GR prefers NR-box 3 to NR-box 2. These results demonstrate that GR prefers binding to NR-box 3 and interacts with an additional GRIP1 site within the CREB (cAMP - response - element binding protein) - binding protein (CBP) binding site.

Example 12: Coactivator peptide binding affinity for TR

To investigate whether the preference of TR for NR-box 2 is dependent on the sequence or structural context of the NR-boxes, competition studies on the interaction of GRIP1 with hTR β LBD were performed using coactivator peptides containing different NR- boxes (NR-box 2 peptide (residues 11-23 of SEQ ID NO: 6) EKHKILHRLQLDS, and NR-box 3 peptide (residues 9-21 of SEQ ID NO: 7) ENALLRYLLDKDD) (Figure 9). Consistent with the interaction of hTR LBD β with GRIP1 (563-767) NR-box mutants, a peptide containing NR-box 1 competes the interaction of GRIP1 with hTR β LBD only at very high concentrations (EC_{50} = 130 μ M). Peptides containing either NR-box 2 or 3 compete GRIP1 (563-767) efficiently and display the preference of hTR β LBD for NR-box 2 (EC_{50} (NR-box 2) = 1.5 μ M, EC_{50} (NR-box 3) = 4 μ M). The apparent affinities (EC_{50}) for peptides of NR-box 2 and 3 are comparable with the analogous GRIP1 (563-767) NR-box mutants suggesting that the preference of TR for NR-boxes is solely dependent on the sequence and independent of the structural context of the NR-boxes.

- 5 Peptides of NR-box 2 or 3 compete GRIP1 (563-767) containing functional NR-boxes 2 and 3 or a mutant of this fragment that contains only a functional NR-box 2 with comparable affinity. Thus, while TR can bind both NR-box 2 and 3, in a GRIP1 coactivator peptide fragment containing both boxes, TR preferentially binds NR-box 2.

These results show the preference of TR for NR-box 2 is sequence dependent.

- 10 The same types of assays for TR competition are performed to assess coactivator peptide binding affinity for GR. The peptide concentrations are normalized relative to TR for obtaining comparable dose response curves.

Example 13: Binding affinity of TR for extended coactivator peptides

- Sequence identity between all three central NR-boxes of the p160 coactivator family is
15 limited to the conserved leucine residues of the (SEQ ID NO: 1) LxxLL motif (**Figure 6**). However, the sequence conservation of a particular NR-box can extend into neighboring residues. To investigate the contribution of these neighboring residues to affinity and specificity of the different NR-boxes for TR, the ability of peptides containing individual NR-boxes with different lengths of adjacent sequences to compete with the interaction of GRIP1 (563-767) with hTR β LBD
20 were compared (**Figure 10**).

- A peptide consisting of the minimal motif of NR-box 3 (residues 12-17 of SEQ ID NO: 7; LLRYLL) does not compete the TR LBD interaction with GRIP1 (563-767). A peptide consisting of the NR-box 2 (residues 15-20 of SEQ ID NO: 6; ILHRLL) also does not sufficiently compete the interaction (data not shown). Extending peptides containing a (SEQ ID NO: 1) LxxLL motif to
25 include adjacent residues increased affinity for both NR-box motifs and magnified the preference of TR for NR-box 2 (NR-box 2 peptides: (residues 11-23 SEQ ID NO: 6) EKHKILHRLLQDS and (residues 7-23 of SEQ ID NO: 6) TSLKEKHKILHRLLQDS; and NR-box 3 peptides: (residues 8-24 of SEQ ID NO: 7) KENALLRYLLDKDDTKD and (residues 5-24 of SEQ ID NO: 7) PKKKENALLRYLLDKDDTKD). A chimeric peptide containing the NR-box 3 motif in the
30 context of the NR-box 2 flanking sequences (SEQ ID NO: 31; TSLKEKHKLLRYLLQDSS) binds like a NR-box 2 peptide.

These results demonstrates that preference of TR for NR-box 2 is at least partially due to features of the bound peptide (residues 15-20 of SEQ ID NO: 6; ILHRLL), but that their affinity and specificity is modulated by adjacent sequences.

5 Example 14: Binding affinity of TR and GR for mutant coactivator

A. TR affinity for ILxxLL motif residues

To investigate the role of the hydrophobic residues in NR-box 2, individual residues of the (residues 15-20 of SEQ ID NO: 6) ILHRL motif were replaced by alanine in the background of GRIP1 (563-767) containing a non-functional NR-box 3 (**Figure 11**). Surprisingly, replacement of
10 any of the conserved leucines prevents binding to TR almost completely. Only replacement of the nonconserved isoleucine exhibited a lessened but still severe impact on the affinity of NR-box 2 for TR. As replacement of a single leucine by alanine is sufficient to overcome the interaction of both the remaining hydrophobic residues and adjacent sequences with hTR β LBD, it appears that their contribution to the affinity of NR-box 2 for hTR β LBD is cooperative rather than additive.

15 Similar results were obtained by competing the interaction of hTR β LBD with the GRIP1 (563-767) NR-box 3 mutant using peptides in which either IL, HR or LL of the NR-box 2 motif are replaced by alanines (**Figure 11**). Whereas the peptides containing the IL or LL replacement failed to interact with the hTR β LBD even at very high concentrations, in agreement with a proposed alpha-helical structure of the motif, replacement of the "HR spacer" by alanines showed a marginal
20 effect on the affinity of the peptide for TR-LBD.

Replacement of single leucine residues of NR-box 2 by phenylalanine reduced the affinity of NR-box 2 peptides for TR LBD about 100-fold, replacement of the isoleucine about 10-fold (**Figure 11**). Therefore, the interaction of TR with GRIP1 relies not simply on the hydrophobicity of the (SEQ ID NO: 1) LxxLL motif, but also on positive contributions by the leucine residues
25 themselves.

These results demonstrate that single mutations of the conserved leucines in the (SEQ ID NO: 1) LxxLL motif strongly reduce affinity of GRIP1 for hTR β LBD.

Collectively, the above examples demonstrate that peptides containing NR-boxes, particularly NR-box 2, reproduce the affinity and specificity of the interaction of GRIP1 (563-767)
30 with hTR β LBD.

B. TR affinity of FxxLW and FxxAL motif residues

The three conserved leucines of the NR-box 2 (SEQ ID NO: 2) ILxxLL motif are embedded in the hydrophobic cleft of the hTR β LBD:NR-box 2 interaction surface, whereas the non conserved

5 isoleucine is located on the rim of this cleft where structural changes can be more easily accommodated (See Example 18). In agreement with this structure, replacement of this residue by alanine or phenylalanine reduced binding to hTR β LBD to a less extent than the comparable mutations of the conserved leucine residues. The surface generated by the three conserved leucines (L690, L693, L694) of the NR-box 2 peptide (residues 12-24 of SEQ ID NO: 6) 686-
10 KHKILHRLQLDSS-698 is highly complementary to the corresponding binding site in the hTR β LBD (Figures 16 and 17). Comparison of this binding site to other nuclear receptors shows that it contains a structural motif that is unique, highly conserved and present in all known structures of nuclear receptor LBDs (Wurtz et al., *Nat Struct Biol.* (1996) 3:87-94; Wagner et al., *supra*; Renaud et al., *Nature* (1995) 378:681-689; Bourguet et al., *Nature* (1995) 375:377-382; and Brzozowski et al., *Nature* (1997) 389:753-758).
15

Interaction of highly conserved hydrophobic motifs, which are part of amphipathic α -helices, with complementary hydrophobic surfaces resembles a feature observed for the interaction of several other transcriptional activators with their target proteins (p53:MDM2, VP16:TAFII31 or CREB:KIX-CBP). However, the motifs of p53 (FxxLW), VP16 (FxxAL) and CREB (YxxIL)
20 differ from the (SEQ ID NO: 1) LxxLL motif of nuclear receptor coactivators. A Fxxxh motif may be generally involved in interaction with TAFII31, where "h" represents any hydrophobic residue. Though with respect to the known structures, complementarity of the interacting hydrophobic surfaces identified here seem to be a common feature of these interactions, cross-reactions between different motifs are possible. For instance, VP16, p53, and p65 (FxxFL) are able to functionally
25 interact with TAFII31, or p53 and E2F1-DP1 (FxxLL) both interact with MDM2. These interactions are sensitive to mutations in the Fxxxh motif. Therefore it appears that either complementarity of the hydrophobic surfaces is not an absolute requirement or that induced fitting of the interacting surfaces is possible.

Based on these observations, studies were performed to determine whether GRIP1 interacts
30 with TAFII31 or MDM2. However, no interaction was detected. GRIP1 mutants changing NR-box 2 (SEQ ID NO: 1; LxxLL) to VP16 (SEQ ID NO: 4; FxxAL) or p53 (SEQ ID NO: 3; FxxLW) like binding sites also failed to bind TAFII31 or MDM2 demonstrating that the presence of the correct binding site is not sufficient to create binding (data not shown). Moreover, peptides containing the VP16 or p53 binding sites are not able to compete the interaction of GRIP1 with TR, even in very
35 high concentration, but do compete the interaction with GR (data not shown). The affinity of this interaction is weak, but comparable to affinity of a peptide of NR-box 2 that, in the context of a

- 5 GRIP1 mutant lacking NR-box 3, binds GR *in vivo* (Ding et al., *supra*). This binding is only about ten times less than a peptide containing NR-box 3, GR's primary binding site.

As shown above, GR binds GRIP1 (563-767) with about one-fifth the affinity than a comparable amount of TR. Thus, the high concentration of NR-box 3 peptide required to compete the interaction of GR with GRIP1 (563-767) may rather reflect a weak affinity of GR for the peptide rather than a particular strong interaction of GR with GRIP1 (563-767).

These results suggest that at least on the peptide level, other hydrophobic motifs besides (SEQ ID NO: 1) LxxLL can interact with the coactivator binding site, but that it is receptor dependent.

C. TR affinity for residues adjacent to ILxxLL motif

- 15 Peptides containing a FxxLL motif bind TR but with two orders of magnitude lower affinity than a (SEQ ID NO: 1) LxxLL motif (Figure 11). To test whether the additional changes in the hydrophobic motif or adjacent sequences of the VP16 peptide prevent its binding to TR, a chimeric peptide containing the NR box-2 motif (SEQ ID NO: 1) LxxLL in the context of the VP16 sequence was constructed. This peptide binds to TR but with an about 100-fold lower affinity than the original NR-box 2 peptide. Thus, the inability to bind the VP16 peptide appears to be due to the combination of an imperfect hydrophobic motif and the incompatibility of TR to adjacent sequences of the VP16 motif.

As the interaction of the chimeric peptide with GR was comparable to the original NR-box 2 and VP16 peptides, this incompatibility appears due to TR-specific features in the NR-box interaction surface. These results show sequences adjacent the NR-box motif LxxLL can reduce binding of NR-box 2 to TR, but not GR.

Example 15: Crystallization and Structure Determination of NR LBD Complexes

A. Crystallization of hTR β LBD with T₃ and GRIP1 NR-box 2 Peptide

- Several peptides containing GRIP1 NR-box 2 were tested in crystallization trials with the hTR β LBD. The complex of the hTR β LBD with the GRIP1 NR-box 2 peptide 686-KHKILHRLQLQDSS-698 (residues 12-24 of SEQ ID NO: 6) produced crystals that were dependent on both the presence and the concentration of the peptide. Without the peptide, the hTR β LBD precipitated immediately. However, nucleation was erratic, but could be overcome through seeding

5 of prepared drops with microcrystals of the hTR β LBD:GRIP1 NR-box 2 peptide complex. Structure of the hTR β LBD:GRIP1 NR-box 2 peptide complex was determined by molecular replacement using the structure of the hTR β LBD determined previously (Wagner et al., *supra*), and refined to a resolution of 3.6Å (Table 1). The refined model consists of residues K211-P254 and V264-D461 of monomer 1 of the hTR β LBD, residues K211-P254 and G261-D461 of monomer 2
10 of the hTR β LBD, and the GRIP1 NR-box 2 peptides (residues 14-24 of SEQ ID NO: 6) 688-KILHRLQLDSS-698, and (residues 14-22 of SEQ ID NO: 6) 688-KILHRLQLD-696 (Appendix 1).

Briefly, the complex between the hTR β LBD and the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) was prepared by mixing (equal)
15 volumes of a solution of 9mg/ml hTR β LBD in 20mM HEPES pH 7.4 with a solution of 14 mM GRIP1 in 0.4mM ammonium acetate pH 4.72, and incubating the mixture on ice for 1 hour. Crystals were obtained after 2 days at 4°C using hanging drop vapor diffusion from a drop containing 1.5µl of hTR β LBD:GRIP1 complex, prepared as described, and 0.5µl 15%PEG 4K, 0.2M sodium citrate pH 4.9, suspended above a reservoir containing 10% PEG 4K, 0.1M
20 ammonium acetate, and 0.05 M sodium citrate (pH 5.6). After allowing the drop to equilibrate for 1 hour, 0.2µl of 10⁻³ to 10⁻⁵ dilutions of microcrystals in reservoir buffer were introduced to provide nucleation. Crystals are of space group P3121 (a=95.2, b=95.2, c=137.6) and contain two molecules of the hTR β LBD and two molecules of the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6).

5

Table 1
Data collection, phasing, and refinement statistics

| Data collection | | | | | | |
|--------------------|------------------|------------------------|----------------|----------------|-------------------------|------------------------|
| Data set | Resolution (Å) | | Reflections | | Coverage (%) | R _{sym} |
| Native | 3.6 | | measured | unique | 96.3 | 0.007 |
| | | | 35565 | 8490 | | |
| Rotation search | | | | | | |
| Search model | Euler angles (°) | | | | Correlation coefficient | |
| | | Θ ₁ | Θ ₂ | Θ ₃ | Highest peak | Highest false peak |
| | hTR β LBD | M1 | 60.12 | 80.68 | 241.90 | 16.3 |
| | M2 | 9.93 | 87.70 | 180.6 | 15.9 | 14.2 |
| Translation search | | | | | | |
| | | Fractional coordinates | | | Translation function | |
| | | x | y | z | Highest peak (o) | Highest false peak (o) |
| | M1 | 0.522 | 0.428 | 0.250 | 19.52 | 10.02 |
| | M2 | 0.200 | 0.932 | 0.119 | 26.11 | 5.77 |
| Refinement | | | | | | |
| | Resolution (Å) | | Reflection | | R | R _{free} |
| F > 2σ | 25 - 3.7 | | 7614 | | 0.2990 | 0.3219 |
| All data | 25 - 3.7 | | 7851 | | 0.3010 | 0.317 |

$R_{sym} = \sum_h \sum_i |I_{hi}| \hat{u} (I_h) / \sum I_h$ for the intensity (I) of i observations of reflection h .

Correlation coefficient = $\sum_h E_o^2 E_c^2 - E_o^2 E_c^2 / [\sum_h (E_o^2 - E_o^2)^2 \sum_h (E_c^2 - E_c^2)^2]^{1/2}$

Translation function (t_a, t_b, \dots) = $\sum_h (|E_o(t_h)|^2 - \sum_h \langle |E_o(t_h)|^2 \rangle) (E_c(t_h, t_a, t_b, \dots))^2 - \langle |E_c(t_h)|^2 \rangle$
 where E_o represents the normalized observed structure factor amplitudes, and E_c represents the normalized structure factors for the search model in a triclinic unit cell with dimensions identical to that of the crystal. The reported peak height represents the value of the function for the translation (t_a, t_b) of the NCS monomers, divided by the rms value of the translation function density.

R factor = $\sum |F_{obs} - F_{calc}| / \sum |F_{obs}|$.

R_{free} is calculated the same as R factor, except only for 10% of the reflections that were set aside for cross validation and not used in refinement.

5 **B. Crystallization of hER α LBD with DES and GRIP1 NR-box 2 Peptide**

Crystals of a DES-hER α LBD-GRIP1 NR-box 2 peptide complex were obtained by hanging drop vapor diffusion. Prior to crystallization, the DES-hER α LBD (residues 297-554) complex was incubated with a 2-4 fold molar excess of the GRIP1 NR-box 2 peptide 686-KHKILHRLQLQDSS-698 (residues 12-24 of SEQ ID NO: 6) for 7-16 hr. Two μ L samples of this solution were mixed
10 with equal volume samples of reservoir buffer consisting of 25-27% (w/v) PEG 4000, 90 mM Tris (pH 8.75-9.0) and 180 mM Na Acetate and suspended over wells containing 800 μ L of the reservoir buffer. After 4-7 days at 19-21°C, rod-like crystals were obtained. The coactivator complex crystals lie in the spacegroup P2₁ with cell dimensions a=54.09, b=82.22, c=58.04 and β =111.34. Two molecules each of the DES-LBD and the coactivator peptide form the asymmetric unit. A 200
15 μ m x 40 μ m x 40 μ m crystal was transferred to a cryosolvent solution containing 25% (w/v) PEG 4000, 10% (w/v) ethylene glycol, 100 mM Tris (pH 8.5), 200 mM Na Acetate and 10 μ M peptide and frozen in an N₂ stream at -170°C in a rayon loop. Diffraction data from this crystal were measured at -170°C using a 300 mm MAR image plate at the Stanford Synchrotron Radiation Laboratory (SSRL) at beamline 7-1 at a wavelength of 1.08 Å. The diffraction images were
20 processed with DENZO and scaled with SCALEPACK (Otwinowski, et al., *Methods Enzymol.* (1997) 276:307-326) using the default -3 σ cutoff.

C. Crystallization of hER α LBD with OHT

Crystals of the hER α LBD (residues 297-554) complexed to OHT were obtained by the hanging drop vapor diffusion method. Equal volume aliquots (2 μ L) of a solution containing 3.9
25 mg/mL protein-ligand complex and the reservoir solution containing 9% (w/v) PEG 8000, 6% (w/v) ethylene glycol, 50 mM HEPES (pH 6.7) and 200 mM NaCl were mixed and suspended over 800 μ L of the reservoir solution. Hexagonal plate-like crystals formed after 4-7 days at 21-23°C. Both crystal size and quality were improved through microseeding techniques. These crystals belong to the space group P6₃22 with cell parameters a=b=58.24 Å and c=277.47 Å. The asymmetric unit
30 consists of a single hER α LBD monomer; the dimer axis lies along a crystallographic two-fold. A single crystal (400 μ m x 250 μ m x 40 μ m) was briefly incubated in a cryoprotectant solution consisting of 10% (w/v) PEG 8000, 25% (w/v) ethylene glycol, 50 mM HEPES (pH 7.0) and 200 mM NaCl and then flash frozen in liquid N₂ suspended in a rayon loop. Diffraction data were measured at -170°C using a 345 mm MAR image plate at SSRL at beamline 9-1 and at a

- 5 wavelength of 0.98 Å. The diffraction images were processed with DENZO and scaled with SCALEPACK (Otwinowski, et al., *supra*) using the default -3σ cutoff.

Example 16: Structure determination and refinement of NR LBD complexes

A. Structure of hTR β LBD with T₃ and GRIP1 NR-box 2 Peptide

- Data were measured using Cu Ka radiation from an R-axis generator at 50 kV and 300 mA
10 with a 0.3mM collimator and a Ni filter. Reflections were measured using an R-Axis II detector and integrated with Denzo, and equivalent reflections scaled using Scalepack (Otwinowski and Minor, "Processing of x-ray diffraction data collected in oscillation mode." In *Macromolecular Crystallography, Part A* (ed. C.W. Carter, Jr. and R.M. Sweet), pp. 307-326. Academic Press, New York, NY). Possible rotation function solutions were calculated using normalized amplitudes in
15 AMORE from a model of hTR β LBD with the ligand, T₃, omitted; translation function solutions were subsequently determined using TFFC for the two rotation solutions with the highest correlation coefficients. For two hTR β LBD molecules in the asymmetric unit, the calculated solvent content is 52%. After rigid body refinement of the two hTR β LBD molecules, electron density maps were calculated. Strong positive density present in both the anomalous and
20 conventional difference Fourier maps for the iodine atoms of the T₃ ligand confirmed the correctness of the solution. The iodine atoms for both T₃ ligands were modeled as a rigid body, and the structure refined with strict NCS symmetry using CNS. Both 2FoFc and FoFc electron density maps showed interpretable density, related by the NCS operator, near H12 of both molecules of the hTR β LBD. The electron density could be modeled as a short α -helix, and the observed side chain
25 density was used to tentatively assign the sequence and direction to the chain. The refined model consists of residues of the hTR β LBD, and peptide residues of the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6).

Atomic coordinates of the hTR β LBD:GRP1 site 2 peptide complex are attached as
Appendix 1.

30 **B. Structure of hER α LBD with DES and GRIP1 NR-box 2 Peptide**

Initial efforts to determine the structure of the DES-hER α LBD-NR box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) complex utilized a low resolution (3.1 Å) data set (data not shown). A self-rotation search implemented with POLARRFN ("The CCP4

5 suite: programs for protein crystallography", *Acta Crystallogr.* (1994) D50:760-763) indicated the presence of a noncrystallographic dyad. The two LBDs in the asymmetric were located by molecular replacement in AMoRe (CCP4, 1994) using a partial polyalanine model of the human RAR γ LBD (Renaud, et al., *supra*) as the search probe (R=58.2%, CC=35.6% after placement of both monomers). Given that the model at this point was both inaccurate (r.m.s.d. 1.7 Å between
10 this model and the final model based on C α positions) and incomplete (accounting for only ~45% of the total scattering matter in the asymmetric unit), an aggressive density modification protocol was undertaken. Iterative cycles of two-fold NCS averaging in DM (CCP4, 1994) interspersed with model building in MOLOC (Muller, et al., *Bull. Soc. Chim. Belg.* (1988) 97:655-667) and model refinement in REFMAC (Murshudov, et al., *Acta Crystallogr.* (1997) D53:240-255) (using tight
15 NCS restraints) were used to quickly build a model of the LBD alone. For this procedure, MAMA (Kleywegt, et al., "Halloween...masks and bones. In From First Map to Final Model", Bailey, et al, eds., Warrington, England, SERC Daresbury Laboratory, 1994) was used for all mask manipulations and PHASES (Furey, et al., PA33 *Am. Cryst. Assoc. Mtg. Abstr.* (1990) 18:73) and the CCP4 suite (CCP4, 1994) were used for the generation of structure factors and the calculation of
20 weights.

However, although the DES-hER α LBD-NR complex model accounted for ~90% of the scattering matter in the asymmetric unit, refinement was being hampered by severe model bias. The high-resolution data set of the DES-hER α LBD-NR-box 2 peptide complex became available when the R_{free} of the OHT-hER α LBD model was ~31%. Both monomers in the asymmetric unit of
25 the DES complex crystal were relocated using AMoRe and the incompletely refined OHT-hER α LBD model (with helix 12 and the loop between helices 11 and 12 removed) as the search model. The missing parts of the model were built and the rest of the model was corrected using MOLOC and two-fold averaged maps generated in DM. Initially, refinement was carried out with REFMAC using tight NCS restraints. At later stages, the model was refined without NCS restraints using the
30 simulated annealing, minimization and B-factor refinement protocols in X-PLOR and a maximum-likelihood target. All B-factors were refined isotropically and anisotropic scaling and a bulk solvent correction were used. The R_{free} set contained a random sample of 6.5% of all data. In refinement, all data between 27 and 2.03 Å (with no σ cutoff) were used. The final model was composed of residues 305-549 of monomer A, residues 305-461 and 470-554 of monomer B, residues 687-697 of
35 peptide A, residues 686-696 of peptide B, 164 waters, two carboxymethyl groups and a chloride ion. According to PROCHECK, 93.7% of all residues in the model were in the core regions of the Ramachandran plot and none were in the disallowed regions. Thus, the structure of the DES-hER α

- 5 LBD-NR-box 2 peptide complex has been refined to a crystallographic R-factor of 19.9% ($R_{\text{free}}=25.0\%$) using data to 2.03 Å resolution.

Ile 689 from the peptide interacts with three receptor residues (Asp 538, Glu 542 and Leu 539). The γ -carboxylate of Glu 542 forms hydrogen bonds to the amides of residues 689 and 690 of the peptide. A water-mediated hydrogen bond network is formed between the imidazole ring of His 377, the γ -carboxylate of Glu 380, and the amide of Tyr 537. Three residues (Glu 380, Leu 536 and Tyr 537) interact with each other through van der Waals contacts and/or hydrogen bonds. Intriguingly, mutations in each these three residues dramatically increase the transcription activity of unliganded ER α LBD (Eng, et al., *Mol. Cell. Biol.* (1997) 17:4644-4653); Lazennec, et al., *Mol. Endocrinol.* (1997) 11:1375-86; White, et al., *EMBO J.* (1997) 16:1427-35). Atomic coordinates of
15 DES-LBD-peptide complex are attached as **Appendix 2**.

5

Table 2

Summary of Crystallographic Statistics

| | | Ligand | |
|----|--|-----------------|--------------------|
| | | DES | OHT |
| | <u>Data Collection</u> | | |
| | Space group | P2 ₁ | P6 ₅ 22 |
| 10 | Resolution | 2.03 | 1.90 |
| | Observations | 104189 | 269253 |
| | Unique | 30265 | 23064 |
| | Completeness (%) | 98.4 | 99.1 |
| | R _{sym} (%) ^a | 7.8 | 7.0 |
| 15 | Average I/σI | 9.8 | 16.1 |
| | <u>Refinement</u> | | |
| | Number of non-hydrogen atoms | 4180 | 2070 |
| | R _{cryst} (%) ^b /R _{free} (%) | 19.9/25.0 | 23.0/26.1 |
| 20 | Bond r.m.s. deviation (Å) | 0.006 | 0.006 |
| | Angle r.m.s. deviation (°) | 1.05 | 1.05 |
| | Average B factor (Å ²) | 34.0 | 40.4 |
| | ^a $R_{\text{sym}} = \sum_i I_i - \langle I_i \rangle / \sum_i I_i$ where $\langle I_i \rangle$ is the average intensity over symmetry equivalents | | |
| 25 | ^b $R_{\text{cryst}} = \sum F_o - F_c / \sum F_o $ | | |

C. Structure of hERα LBD-OHT complex

The OHT complex data set was then collected. Starting with one of the monomers of the preliminary low-resolution DES-hERα LBD-NR-box 2 peptide model as the search probe, molecular replacement in AMoRe was used to search for the location of LBD in this crystal form in both P6₁22 and P6₅22. A translation search in P6₅22 yielded the correct solution (R=53.8%, CC=38.2%). In order to reduce model bias, DMMULTI (CCP4, 1994) was then used to project averaged density from the DES complex cell into the OHT complex cell. Using MOLOC, a model of the hERα LBD was built into the resulting density. The model was refined initially in REFMAC and later with the simulated annealing, positional and B-factor refinement protocols in X-PLOR

5 (Brunger, X-PLOR Version 3.843, New Haven, Connecticut: Yale University, 1996) using a maximum-likelihood target (Adams, et al., *Proc. Natl. Acad. Sci. USA* (1997) 94:5018-23). Anisotropic scaling and a bulk solvent correction were used and all B-factors were refined isotropically. Except for the R_{free} set (a random sampling consisting of 8% of the data set), all data between 41 and 1.9 Å (with no σ cutoff) were included. The final model consisted of residues 306-10 551, the ligand and 78 waters. According to PROCHECK (CCP4, 1994), 91.6% of all residues in the model were in the core regions of the Ramachandran plot and none were in the disallowed regions. Thus, the structure of the OHT-hER α LBD complex has been refined against data of comparable resolution (1.90 Å) to a crystallographic R-factor of 23.0% (R_{free} =26.2%). Atomic coordinates of OHT-hER α LBD complex are attached as **Appendix 3**.

15 **Example 17: Structural analysis of hTR β LBD:GRIP 1 NR-box 2 peptide complex**

A. Structure of cocrystal complex (contents of asu)

The asymmetric unit (asu) of the crystal contains two monomers of the hTR β LBD and two molecules of the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6), which observes the NCS relation of the two TR monomers (**Figure 12**). The structure of the hTR β LBD, which closely resembles that of the rTR α LBD (Wagner et al., *supra*), consists of twelve alpha-helices and two β -strands organized in three layers, resembling an alpha-helical sandwich. The only significant difference between the hTR β LBD and the rTR α LBD is disorder in the loop between helices H1 and H3. The GRIP1 NR-box 2 peptide forms an amphipathic α -helix of about 3 turns, preceded by 2 residues and followed by 3 residues in extended coil conformation.

25 The relation of the two monomers of the hTR β LBD is primarily translational, and does not resemble the homodimer structures reported for the hRXR, or the hER (Bourguet et al., *supra*; Brzozowski et al., *supra*). Furthermore, the interface between the two monomers does not involve residues necessary for formation of the physiological TR dimer. Instead, one of the cocrystal peptides appears to bridge the interaction between the two monomers. The hydrophobic face of the alpha-helix of the cocrystal peptide contacts monomer 1 of the hTR β LBD at H3, H5, and H12, while the hydrophilic face contacts monomer 2 at the hairpin turn preceding strand S3. The second cocrystal peptide also contacts monomer 2 at H3, H5, and H12, and the two cocrystal peptides observe the same NCS relation as TR LBD monomers.

5 The common interface between both cocrystal peptides and the hTR β LBD buries the hydrophobic residues that define the cocrystal peptide (SEQ ID NO: 1) LxxLL sequence motif, residues Ile689, Leu690, Leu693, and Leu694; against the surface of the receptor LBD (Figures 16 and 17). The presence of the second peptide in the crystal, duplicating the interactions of the hydrophobic residues, suggests those interactions are specific and drive the interaction of the peptide with the hTR β LBD, while the hydrophilic interactions provide a fortuitous crystal contact and account for the dependence of crystallization on the presence and concentration of the peptide.

B. Structure of the GRIP1 NR-box 2 peptide

15 The GRIP1 NR-box 2 peptide used in the crystallization is 13 amino acids long (residues 12-24 of SEQ ID NO: 6; 686-KHKILHRLQLDSS-698). For the NR-box 2 peptide in monomer 1 (peptide 1), 12 amino acids are ordered in the crystal. Residues K688 - Q694 form an amphipathic helix, with residues K686-H687 and D695-S698 on either end in extended coil conformations. For the NR-box 2 peptide in monomer 2 (peptide 2), residues K688 - Q694 again form an amphipathic helix, but the ends of the peptide are disordered. While the resolution of the current data prevents absolute assignment of hydrogen bonds, it is evident from the periodicity of the side chain density that the central residues form an alpha-helix. In the absence of TR the far UV-CD spectrum of the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) appears to be random coil (data not shown). Stable helix formation may thus be induced by the interaction of the hydrophobic amino acids with the receptor LBD as it has been proposed in other protein:protein interactions, such as p53:MDM2 (Kussie et al., *Science* (1996) 274:948-953), VP16:TAF31 (Uesugi et al., *Science* (1996) 277:1310-1313), and CREB:KIX-CBP (Radhakrishnan et al., *Cell* (1997) 91:741-752).

C. Structure of the hTR β LBD:GRIP1 NR-box 2 peptide interface

30 The hTR β LBD of the cocrystal contributes residues from three helices, H3, H5, and H12 to the interface, which pack against one another to create a hydrophobic cleft. The residues lining the cleft are I280, T281, V283, V284, A287, and K288 from H3; Q301, I302, L305, and K306 from H5; and L454, E457, V458, and F459 from H12. A cysteine residue (C309) from H6 appears to provide a partial surface that is buried deep within the bottom of the cleft.

 The GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) binds at the junction of H3 and H12. Leu690 of the bound peptide inserts into a shallow but

5 defined depression at the base of the cleft, making van der Waals contact with L454 and V458 of H12, while peptide residue Ile689 packs against L454 of H12 outside the edge of the cleft; L454, then, interdigitates between the two residues. One further turn C-terminal along the alpha-helix, L693 and L694 of the bound peptide pack into complementary pockets within the hydrophobic cleft. Peptide residue L693 forms van der Waals contact with V284 of H3, while peptide residue
10 L694, bound more deeply in the cleft, makes contact with F298 and L305 of H4 and H5. The hydrophobic interactions of the GRIP1 NR-box 2 peptide with the hTR β LBD are observed for both cocrystal peptides 1 and 2 in their respective monomers of the crystal dimer complex, suggesting that the interactions are specific to the peptide, and not induced by crystallization.

Example 18: Overall Structure of the DES-hER α -LBD-NR-box 2 Peptide Complex

15 The asymmetric unit of the DES-hER α LBD-NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) complex crystals contains the same noncrystallographic dimer of LBDs that has been observed in the previously determined structures of the LBD bound to both E₂ and RAL (Brzozowski, et al., *supra* and Tanenbaum, et al., *supra*). Beyond the flexible loops between helices 2 and 3 and helices 9 and 10, the two LBDs of the dimer adopt similar
20 structures (r.m.s.d. 0.47 Å based on C α positions). The conformation of each LBD complexed with DES closely resembles that of the LBD bound to E₂ (Brzozowski, et al., *supra*); each monomer is a wedge shaped molecule consisting of three layers of eleven to twelve helices and a single beta hairpin. In each LBD, the hydrophobic face of helix 12 is packed against helices 3, 5/6 and 11 covering the ligand binding pocket. One NR-box 2 peptide is bound to each LBD in a hydrophobic
25 cleft composed of residues from helices 3, 4, 5 and 12 and the turn between 3 and 4. The density for both peptides in the asymmetric unit is continuous and unambiguous. Residues 687 to 697 from peptide A and residues 686 to 696 from peptide B have been modeled; the remaining residues are disordered. Given that each peptide lies within a different environment within the crystal, it is striking that from residues Ile 689 to Gln 695 each peptide forms a two turn, amphipathic α helix.
30 Flanking this region of common secondary structure, the peptides adopt dissimilar random coil conformations.

Example 19: Structure of the OHT-hER α LBD Complex

The binding of OHT induces a conformation of the hER α LBD that differs in both secondary and tertiary structural organization from that driven by DES binding. In the DES

5 complex, the main chain from residues 339 to 341, 421 to 423, and 527 to 530 form parts of helices 3, 8 and 11 respectively. In contrast, these regions adopt an extended conformation in the OHT complex. In addition, the composition and orientation of helix 12 are different in the two structures. Helix 12 in the DES complex consists of residues 538 to 546 whereas helix 12 in the OHT complex consists of residues 536 to 544. Most dramatically, rather than covering the ligand binding pocket
10 as it does in the DES complex, helix 12 in the OHT complex occupies the part of the coactivator binding groove formed by residues from helices 3, 4, and 5, and the turn connecting helices 3 and 4. This alternative conformation of helix 12 appears to be similar to that observed in the RAL complex (Brzozowski, et al., *supra*).

Example 20: Coactivator binding site structure and function

15 A. TR coactivator binding site

The above examples demonstrate that nuclear receptors, exemplified by TR, GR and ER, are recognized by specific coactivators that bind thereto through a coupling surface comprising a hydrophobic cleft and a charged hydrophobic perimeter. Identification and characterization of this coupling surface and the coactivator binding site of nuclear receptors offers a new target for the
20 design and selection of compounds that modulate binding of coactivator to nuclear receptors.

Residues forming the coactivator binding site were found to cluster within a surprisingly small area with well-defined borders (see, e.g., **Figures 5, 14, and 15**). As is shown in above Examples, mutated residues nearby this area do not affect coactivator binding or transcriptional activation. Additionally, the coactivator binding assays and structural analyses demonstrated that
25 NR-box containing proteins and peptides bind to this site. These results also showed that the GRIP1 coactivator protein binds to the site through a highly (SEQ ID NO: 1) LxxLL.

The structural analyses showed that residues contacting a conserved leucine residue of the (SEQ ID NO: 1) LxxLL motif included V284, F293, I302, L305 and L454. Residues within 4.5Å of an atom of the bound peptide included T281, V284, K288, F293, Q301, I302, L305, K306, P453,
30 L454 and E457. Structural analyses also revealed two other features of the site: a hydrophobic residue from helix 12 (Phe459) that contributes to local packing, and a cysteine residue contributed by helix 6 (Cys309) that provides a partial surface buried deep within the site. Mutational analyses showed that residues which block GRIP1 and SRC-1 coactivator binding when mutated are residues V284, K288, I302, K306, L454, and V458. Mutated residues likely to undergo a conformational
35 change upon hormone binding included Leu454 and Glu457. Thus, the site identified by

5 mutational, binding assays and crystallography corresponds to a surprisingly small cluster of residues on the surface of the LBD that define a prominent hydrophobic cleft formed by hydrophobic residues corresponding to human TR residues of C-terminal helix 3 (Ile280, Val283, Val284, and Ala287), helix 4 (Phe293), helix 5 (Ile302 and Leu305), helix 6 (Cys309), and helix 12 (Leu454, Val458 and Phe459). Collectively, the Examples indicate that residues forming the site
10 are amino acids corresponding to human TR residues of C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459). The coactivator binding site is highly conserved among the nuclear receptor super family (**Figure 19**).

The coactivator binding site of TR contains charged and hydrophobic residues at its
15 periphery, but only hydrophobic residues at its center (see, e.g., **Figures 5 and 18**). The hydrophobic cleft at the center of the site may play a significant role in driving the coactivator binding reaction. The site is comprised of two parts (**Figure 18**), right). Residues contained in helices 3, 5 and 6 (**Figure 18**, yellow residues) likely form a constitutive part, since their positions are identical in all nuclear receptor structures reported, including the liganded, activated states of
20 the TR, RAR, and ER, the unliganded RXR, and the inhibitor-liganded ER. By contrast, the residues of helix 12 (**Figure 18**, red residues) are differently positioned in the active and inactive states reported. Thus the coactivator binding site for the nuclear receptors is likely to be formed in response to an active hormone by positioning helix 12 against a scaffold formed by helices 3-6. Because the coactivator binding site is so small, it is easy to understand how even slight changes in
25 the position of helix 12, which may, for example, be induced by an antagonist ligand, could impair coactivator binding, and thus receptor activation.

B. ER coactivator binding site

Binding of the NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) to the ER α LBD buries 1000 Å² of predominantly hydrophobic surface area from both
30 molecules. The NR-box 2 peptide binding site is a shallow groove composed of residues Leu 354, Val 355, Ile 358, Ala 361 and Lys 362 from helix 3; Phe 367 and Val 368 from helix 4; Leu 372 from the turn between helices 3 and 4; Gln 375, Val 376, Leu 379 and Glu 380 from helix 5; and Asp 538, Leu 539, Glu 542 and Met 543 from helix 12. The floor and sides of this groove are completely nonpolar, but the ends of this groove are charged. Therefore, structural characterization
35 of the binding site of the NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) to the ER α LBD, which is the same NR-box 2 peptide utilized to crystallize the T₃-TR

5 LBD, supports the findings for TR that residues forming the coactivator binding site of nuclear
receptors is composed of a well defined hydrophobic cleft and a charged hydrophobic perimeter.
These residues are highly conserved among the nuclear receptor super family (Figure 19).
Structural characterization of the coactivator peptide-bound ER LBD also supports the concept of
exploiting the slight differences among the coactivator binding sites of nuclear receptors in
10 designing and identifying compounds that target specific nuclear receptors.

The ER α LBD interacts primarily with the hydrophobic face of the NR-box 2 peptide 686-
KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) α helix formed by the side chains of
Ile 689 and the three (SEQ ID NO: 1) LxxLL motif leucines (Leu 690, Leu 693 and Leu 694). The
side chain of Leu 690 is deeply embedded within the groove and forms van der Waals contacts with
15 the side chains of Ile 358, Val 376, Leu 379, Glu 380 and Met 543. The side chain of Leu 694 is
similarly isolated within the groove and makes van der Waals contacts with the side chains of Ile
358, Lys 362, Leu 372, Gln 375, Val 376 and Leu 379. In contrast, the side chains of both Ile 689
and the second NR box leucine, Leu 693, rest against the rim of the groove. The side chain of Ile
689 lies in a shallow depression formed by the side chains of Asp 538, Leu 539 and Glu 542. The
20 side chain of Leu 693 makes nonpolar contacts with the side chains of Ile 358 and Leu 539.

The charged and polar side chains which form the hydrophilic face of the peptide helix
project away from the ER α receptor and either interact predominantly with solvent or form
symmetry contacts. None of the side chains of the polar and charged residues outside the helical
region of either peptide in the asymmetric unit, with the exception of Lys 688 of peptide B, is
25 involved in hydrogen bonds or salt bridges with its associated ER α LBD monomer. The ϵ -amino
group of Lys 688 of peptide B hydrogen bonds to the side chain carboxylate of Glu 380 of
monomer B. This interaction is presumably a crystal artifact; the main chain atoms of the N-
terminal three residues of peptide B are displaced from monomer B and interact extensively with a
symmetry-related ER α LBD.

30 In addition to interacting with the hydrophobic face of the peptide helix, the ER α LBD
stabilizes the main chain conformation of the NR box peptide by forming capping interactions with
both ends of the peptide helix. Glu 542 and Lys 362 are positioned at opposite ends of the peptide
binding site. The side chains of Glu 542 and Lys 362 form van der Waals contacts with main chain
and side chain atoms at the N- and C-terminal turns of the peptide helix respectively. These
35 interactions position the stabilizing charges of the γ -carboxylate of Glu 542 and ϵ -amino group of
Lys 362 near the ends of the NR box peptide helix. The side chain carboxylate of Glu 542

- 5 hydrogen bonds to the amides of the residues of N-terminal turn of the peptide helix (residues 688 and 689 of peptide A; residues 689 and 690 of peptide B). Similarly, the ϵ -amino group of Lys 362 hydrogen bonds to the carbonyls of the residues of the C-terminal turn of the peptide helix (residue 693 of peptide A; residues 693 and 694 of peptide B).

- 10 Except for the orientation of helix 12, the structure of the peptide binding groove of the ER α LBD is almost identical in the DES and OHT complexes. The region of this groove outside of helix 12 is referred to herein as the "static region" of the NR box binding site. Helix 12 in the OHT complex and the NR box peptide helix in the DES complex interact with the static region of the coactivator recognition groove in strikingly similar ways.

- 15 Helix 12 mimics the hydrophobic interactions of the NR box peptide with the static region of the groove with a stretch of residues (residues 540 to 544) that resembles an NR box ((residues 6-10 of SEQ ID NO: 43) LLEML instead of (SEQ ID NO: 1) LxxLL). The side chains of Leu 540 and Met 543 lie in approximately the same locations as those of the first and second motif leucines (Leu 690 and Leu 693) in the peptide complex. Leu 540 is inserted into the groove and makes van der Waals contacts with Leu 354, Val 376 and Glu 380. Met 543 lies along the edge of the groove and forms van der Waals contacts with the side chains of Leu 354, Val 355 and Ile 358. The side chain position of Leu 544 almost exactly overlaps that of the third NR box leucine, Leu 694. Deep within the groove, the Leu 544 side chain makes van der Waals contacts with the side chains of Ile 358, Lys 362, Leu 372, Gln 375, Val 376 and Leu 379.

- 25 Helix 12 in the OHT complex is also stabilized by N- and C-terminal capping interactions. Lys 362 interacts with the C-terminal turn of helix 12 much as it does with the equivalent turn of the peptide helix. The Lys 362 side chain packs against the C-terminal turn of the helix 12 with its ϵ -amino group hydrogen bonding to the carbonyls of residues 543 and 544. Given that the capping interaction at the N-terminal turn coactivator helix is formed by a helix 12 residue (Glu 542), the N-terminal turn of helix 12 in the antagonist complex is forced to interact with another residue, Glu 380. The Glu 380 γ -carboxylate forms van der Waals contacts with Tyr 537 and interacts with the amide of Tyr 537 through a series of water-mediated hydrogen bonds.

- 35 In addition to forming these "NR box-like" interactions, helix 12 also forms van der Waals contacts with areas of the ER α LBD outside of the coactivator recognition groove. The side chain of Leu 536 forms van der Waals contacts with Glu 380 and Trp 383 and that of Tyr 537 forms van der Waals contacts with His 373, Val 376 and Glu 380. As a result of these contacts, helix 12 in the

- 5 OHT complex buries more solvent accessible surface area ($\sim 1200 \text{ \AA}^2$) than the NR box peptide in the DES-ER α LBD-peptide complex.

Identification and characterization of the coactivator binding site for TR, and extension of this information to other nuclear receptors shows that this site is common for all nuclear receptors identified to date. Additionally, sequence and structural comparison, coupled with the Examples showing differential specificity for coactivator binding to TR, GR and ER, reveal that minor differences between the receptors, such as found in helix 12, are likely to influence specificity of a coactivator for different types of nuclear receptors. Thus, the Examples presented herein demonstrate that information derived from the structure and function of the TR coactivator binding site can be applied in design and selection of compounds that modulate binding of coactivator proteins to nuclear receptors for all members of the nuclear receptor super family.

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All publications and patent applications mentioned in this specification are herein incorporated by reference to the same extent as if each individual publication or patent application was specifically and individually indicated to be incorporated by reference.

30 The invention now being fully described, it will be apparent to one of ordinary skill in the art that many changes and modifications can be made thereto without departing from the spirit or scope of the appended claims.

5

Appendix 1

Atomic Coordinates for Human TR- β Complexed With T₃, and a GRIP1 NR-box 2 Peptide

| | | | | | | | | | | |
|----|--------|---|-----|-----------|--------|--------|--------|------|-------|---|
| | REMARK | full length numbering | | | | | | | | |
| 10 | REMARK | all residue names correct | | | | | | | | |
| | REMARK | peptide sequence | | | | | | | | |
| | REMARK | two molecules of TRB - CHAIN A and CHAIN B | | | | | | | | |
| | REMARK | two molecules of T3 - CHAIN J and CHAIN K | | | | | | | | |
| | REMARK | two molecules of GRIP-1 peptide - CHAIN X and CHAIN Y | | | | | | | | |
| 15 | REMARK | chain X lies between A and B | | | | | | | | |
| | REMARK | chain Y interacts with B only | | | | | | | | |
| | REMARK | residues differing between A and B include: | | | | | | | | |
| | REMARK | A 217 Glu, A 252 Gln, A 263 Lys (missing side chains) | | | | | | | | |
| | REMARK | B 237 Ser, B239 His, B 394 Lys (missing side chains) | | | | | | | | |
| 20 | REMARK | additionally Gly 261, Gly 262 are not visible in chain A | | | | | | | | |
| | REMARK | residues differing between X and Y include: | | | | | | | | |
| | REMARK | A 692 Arg | | | | | | | | |
| | REMARK | additionally, residues Lys 688, Lys 689; Ser 697, Ser 698 | | | | | | | | |
| | REMARK | are not visible in chain Y | | | | | | | | |
| 25 | ATOM | 1 | N | LYS A 211 | 52.546 | 23.912 | 35.239 | 1.00 | 45.76 | 7 |
| | ATOM | 2 | CA | LYS A 211 | 52.944 | 24.345 | 36.586 | 1.00 | 43.42 | 6 |
| | ATOM | 3 | C | LYS A 211 | 52.035 | 23.665 | 37.836 | 1.00 | 35.68 | 6 |
| | ATOM | 4 | O | LYS A 211 | 51.511 | 22.556 | 37.763 | 1.00 | 33.58 | 8 |
| | ATOM | 5 | CB | LYS A 211 | 52.610 | 25.825 | 36.779 | 1.00 | 46.72 | 6 |
| 30 | ATOM | 6 | N | PRO A 212 | 51.678 | 24.182 | 39.199 | 1.00 | 35.64 | 7 |
| | ATOM | 7 | CD | PRO A 212 | 52.082 | 25.474 | 39.842 | 1.00 | 38.60 | 6 |
| | ATOM | 8 | CA | PRO A 212 | 50.809 | 23.379 | 40.166 | 1.00 | 38.35 | 6 |
| | ATOM | 9 | CB | PRO A 212 | 50.670 | 24.194 | 41.440 | 1.00 | 38.95 | 6 |
| | ATOM | 10 | CG | PRO A 212 | 51.455 | 25.469 | 41.255 | 1.00 | 42.00 | 6 |
| 35 | ATOM | 11 | C | PRO A 212 | 49.433 | 23.097 | 39.594 | 1.00 | 38.78 | 6 |
| | ATOM | 12 | O | PRO A 212 | 48.920 | 23.949 | 38.802 | 1.00 | 34.64 | 8 |
| | ATOM | 13 | N | GLU A 213 | 48.901 | 21.948 | 40.014 | 1.00 | 40.31 | 7 |
| | ATOM | 14 | CA | GLU A 213 | 47.609 | 21.419 | 39.529 | 1.00 | 43.87 | 6 |
| | ATOM | 15 | CB | GLU A 213 | 47.943 | 20.307 | 38.520 | 1.00 | 45.16 | 6 |
| 40 | ATOM | 16 | CG | GLU A 213 | 49.125 | 20.708 | 37.601 | 1.00 | 47.60 | 6 |
| | ATOM | 17 | CD | GLU A 213 | 49.284 | 19.828 | 36.353 | 1.00 | 50.68 | 6 |
| | ATOM | 18 | OE1 | GLU A 213 | 49.355 | 18.547 | 36.474 | 1.00 | 59.18 | 8 |
| | ATOM | 19 | OE2 | GLU A 213 | 49.356 | 20.368 | 35.180 | 1.00 | 49.06 | 8 |
| | ATOM | 20 | C | GLU A 213 | 46.711 | 20.988 | 40.747 | 1.00 | 45.96 | 6 |
| 45 | ATOM | 21 | O | GLU A 213 | 47.111 | 21.136 | 41.910 | 1.00 | 43.13 | 8 |
| | ATOM | 22 | N | PRO A 214 | 45.463 | 20.460 | 40.515 | 1.00 | 46.52 | 7 |
| | ATOM | 23 | CD | PRO A 214 | 44.985 | 20.184 | 39.148 | 1.00 | 46.44 | 6 |
| | ATOM | 24 | CA | PRO A 214 | 44.447 | 20.124 | 41.596 | 1.00 | 47.52 | 6 |
| | ATOM | 25 | CB | PRO A 214 | 43.249 | 19.629 | 40.816 | 1.00 | 45.40 | 6 |
| 50 | ATOM | 26 | CG | PRO A 214 | 43.588 | 19.674 | 39.327 | 1.00 | 49.89 | 6 |
| | ATOM | 27 | C | PRO A 214 | 44.787 | 19.082 | 42.625 | 1.00 | 45.70 | 6 |
| | ATOM | 28 | O | PRO A 214 | 45.816 | 18.466 | 42.535 | 1.00 | 44.49 | 8 |
| | ATOM | 29 | N | THR A 215 | 43.915 | 18.876 | 43.606 | 1.00 | 45.24 | 7 |
| | ATOM | 30 | CA | THR A 215 | 44.161 | 17.890 | 44.686 | 1.00 | 49.36 | 6 |
| 55 | ATOM | 31 | CB | THR A 215 | 44.163 | 18.586 | 46.093 | 1.00 | 44.86 | 6 |
| | ATOM | 32 | OG1 | THR A 215 | 42.878 | 18.447 | 46.728 | 1.00 | 52.26 | 8 |
| | ATOM | 33 | CG2 | THR A 215 | 44.514 | 20.031 | 45.974 | 1.00 | 39.43 | 6 |
| | ATOM | 34 | C | THR A 215 | 42.934 | 16.995 | 44.667 | 1.00 | 52.51 | 6 |

| | | | | | | | | | | | | |
|----|------|----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 35 | O | THR | A | 215 | 41.816 | 17.501 | 44.691 | 1.00 | 53.48 | 8 |
| | ATOM | 36 | N | ASP | A | 216 | 43.118 | 15.683 | 44.607 | 1.00 | 58.81 | 7 |
| | ATOM | 37 | CA | ASP | A | 216 | 41.973 | 14.740 | 44.615 | 1.00 | 61.51 | 6 |
| | ATOM | 38 | CB | ASP | A | 216 | 42.386 | 13.451 | 45.343 | 1.00 | 70.57 | 6 |
| | ATOM | 39 | CG | ASP | A | 216 | 42.399 | 12.283 | 44.475 | 1.00 | 78.07 | 6 |
| 10 | ATOM | 40 | OD1 | ASP | A | 216 | 41.532 | 12.161 | 43.586 | 1.00 | 82.31 | 8 |
| | ATOM | 41 | OD2 | ASP | A | 216 | 43.293 | 11.436 | 44.684 | 1.00 | 86.55 | 8 |
| | ATOM | 42 | C | ASP | A | 216 | 40.640 | 15.311 | 45.268 | 1.00 | 58.42 | 6 |
| | ATOM | 43 | O | ASP | A | 216 | 39.598 | 14.840 | 44.924 | 1.00 | 56.85 | 8 |
| | ATOM | 44 | N | GLU | A | 217 | 40.673 | 16.270 | 46.217 | 1.00 | 54.92 | 7 |
| 15 | ATOM | 45 | CA | GLU | A | 217 | 39.502 | 16.937 | 46.856 | 1.00 | 53.37 | 6 |
| | ATOM | 46 | CB | GLU | A | 217 | 39.943 | 17.459 | 48.216 | 1.00 | 51.02 | 6 |
| | ATOM | 47 | C | GLU | A | 217 | 39.113 | 18.144 | 45.956 | 1.00 | 53.55 | 6 |
| | ATOM | 48 | O | GLU | A | 217 | 37.905 | 18.394 | 45.695 | 1.00 | 54.33 | 8 |
| | ATOM | 49 | N | GLU | A | 218 | 40.162 | 18.895 | 45.511 | 1.00 | 49.20 | 7 |
| 20 | ATOM | 50 | CA | GLU | A | 218 | 39.933 | 20.073 | 44.661 | 1.00 | 45.94 | 6 |
| | ATOM | 51 | CB | GLU | A | 218 | 41.232 | 20.855 | 44.304 | 1.00 | 43.43 | 6 |
| | ATOM | 52 | CG | GLU | A | 218 | 41.907 | 21.579 | 45.479 | 1.00 | 40.86 | 6 |
| | ATOM | 53 | CD | GLU | A | 218 | 43.061 | 22.446 | 45.074 | 1.00 | 39.88 | 6 |
| | ATOM | 54 | OE1 | GLU | A | 218 | 43.895 | 22.019 | 44.232 | 1.00 | 37.61 | 8 |
| 25 | ATOM | 55 | OE2 | GLU | A | 218 | 43.183 | 23.583 | 45.599 | 1.00 | 34.01 | 8 |
| | ATOM | 56 | C | GLU | A | 218 | 39.249 | 19.647 | 43.390 | 1.00 | 44.71 | 6 |
| | ATOM | 57 | O | GLU | A | 218 | 38.302 | 20.291 | 42.964 | 1.00 | 45.31 | 8 |
| | ATOM | 58 | N | TRP | A | 219 | 39.720 | 18.553 | 42.797 | 1.00 | 44.02 | 7 |
| | ATOM | 59 | CA | TRP | A | 219 | 39.109 | 18.061 | 41.574 | 1.00 | 46.97 | 6 |
| 30 | ATOM | 60 | CB | TRP | A | 219 | 39.799 | 16.793 | 41.074 | 1.00 | 48.42 | 6 |
| | ATOM | 61 | CG | TRP | A | 219 | 40.879 | 17.029 | 40.141 | 1.00 | 54.61 | 6 |
| | ATOM | 62 | CD2 | TRP | A | 219 | 40.755 | 17.256 | 38.733 | 1.00 | 55.24 | 6 |
| | ATOM | 63 | CE2 | TRP | A | 219 | 42.067 | 17.523 | 38.245 | 1.00 | 53.67 | 6 |
| | ATOM | 64 | CE3 | TRP | A | 219 | 39.691 | 17.234 | 37.828 | 1.00 | 54.55 | 6 |
| 35 | ATOM | 65 | CD1 | TRP | A | 219 | 42.159 | 17.159 | 40.447 | 1.00 | 55.75 | 6 |
| | ATOM | 66 | NE1 | TRP | A | 219 | 42.895 | 17.485 | 39.339 | 1.00 | 54.43 | 7 |
| | ATOM | 67 | CZ2 | TRP | A | 219 | 42.330 | 17.851 | 36.895 | 1.00 | 52.54 | 6 |
| | ATOM | 68 | CZ3 | TRP | A | 219 | 39.943 | 17.535 | 36.509 | 1.00 | 55.17 | 6 |
| | ATOM | 69 | CH2 | TRP | A | 219 | 41.239 | 17.820 | 36.029 | 1.00 | 55.59 | 6 |
| 40 | ATOM | 70 | C | TRP | A | 219 | 37.646 | 17.743 | 41.812 | 1.00 | 47.32 | 6 |
| | ATOM | 71 | O | TRP | A | 219 | 36.788 | 18.028 | 40.978 | 1.00 | 43.56 | 8 |
| | ATOM | 72 | N | GLU | A | 220 | 37.376 | 17.142 | 42.965 | 1.00 | 49.91 | 7 |
| | ATOM | 73 | CA | GLU | A | 220 | 36.021 | 16.769 | 43.316 | 1.00 | 53.57 | 6 |
| | ATOM | 74 | CB | GLU | A | 220 | 36.052 | 16.055 | 44.649 | 1.00 | 58.18 | 6 |
| 45 | ATOM | 75 | CG | GLU | A | 220 | 35.149 | 14.930 | 44.672 | 1.00 | 73.13 | 6 |
| | ATOM | 76 | CD | GLU | A | 220 | 35.735 | 13.935 | 45.442 | 1.00 | 80.06 | 6 |
| | ATOM | 77 | OE1 | GLU | A | 220 | 36.886 | 13.575 | 45.173 | 1.00 | 82.12 | 8 |
| | ATOM | 78 | OE2 | GLU | A | 220 | 35.078 | 13.478 | 46.378 | 1.00 | 82.78 | 8 |
| | ATOM | 79 | C | GLU | A | 220 | 35.161 | 18.026 | 43.381 | 1.00 | 50.51 | 6 |
| 50 | ATOM | 80 | O | GLU | A | 220 | 33.991 | 18.010 | 42.995 | 1.00 | 49.94 | 8 |
| | ATOM | 81 | N | LEU | A | 221 | 35.761 | 19.120 | 43.865 | 1.00 | 43.71 | 7 |
| | ATOM | 82 | CA | LEU | A | 221 | 35.047 | 20.398 | 43.951 | 1.00 | 42.81 | 6 |
| | ATOM | 83 | CB | LEU | A | 221 | 35.935 | 21.510 | 44.510 | 1.00 | 39.21 | 6 |
| | ATOM | 84 | CG | LEU | A | 221 | 35.375 | 22.908 | 44.353 | 1.00 | 36.34 | 6 |
| 55 | ATOM | 85 | CD1 | LEU | A | 221 | 33.941 | 22.929 | 44.836 | 1.00 | 36.93 | 6 |
| | ATOM | 86 | CD2 | LEU | A | 221 | 36.226 | 23.910 | 45.122 | 1.00 | 24.18 | 6 |
| | ATOM | 87 | C | LEU | A | 221 | 34.563 | 20.815 | 42.575 | 1.00 | 43.46 | 6 |
| | ATOM | 88 | O | LEU | A | 221 | 33.392 | 21.104 | 42.395 | 1.00 | 45.25 | 8 |

| | | | | | | | | | | | | |
|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 89 | N | ILE | A | 222 | 35.498 | 20.871 | 41.628 | 1.00 | 39.09 | 7 |
| | ATOM | 90 | CA | ILE | A | 222 | 35.192 | 21.226 | 40.254 | 1.00 | 35.47 | 6 |
| | ATOM | 91 | CB | ILE | A | 222 | 36.379 | 20.997 | 39.343 | 1.00 | 33.74 | 6 |
| | ATOM | 92 | CG2 | ILE | A | 222 | 35.970 | 21.182 | 37.893 | 1.00 | 28.86 | 6 |
| | ATOM | 93 | CG1 | ILE | A | 222 | 37.532 | 21.922 | 39.707 | 1.00 | 33.33 | 6 |
| 10 | ATOM | 94 | CD1 | ILE | A | 222 | 38.804 | 21.586 | 39.004 | 1.00 | 34.85 | 6 |
| | ATOM | 95 | C | ILE | A | 222 | 34.067 | 20.365 | 39.735 | 1.00 | 34.26 | 6 |
| | ATOM | 96 | O | ILE | A | 222 | 33.033 | 20.873 | 39.319 | 1.00 | 31.90 | 8 |
| | ATOM | 97 | N | LYS | A | 223 | 34.301 | 19.058 | 39.750 | 1.00 | 39.49 | 7 |
| | ATOM | 98 | CA | LYS | A | 223 | 33.316 | 18.100 | 39.276 | 1.00 | 44.43 | 6 |
| 15 | ATOM | 99 | CB | LYS | A | 223 | 33.603 | 16.713 | 39.852 | 1.00 | 50.81 | 6 |
| | ATOM | 100 | CG | LYS | A | 223 | 32.741 | 15.631 | 39.227 | 1.00 | 62.51 | 6 |
| | ATOM | 101 | CD | LYS | A | 223 | 32.859 | 14.291 | 39.943 | 1.00 | 72.22 | 6 |
| | ATOM | 102 | CE | LYS | A | 223 | 31.798 | 13.318 | 39.430 | 1.00 | 74.55 | 6 |
| | ATOM | 103 | NZ | LYS | A | 223 | 31.900 | 11.985 | 40.106 | 1.00 | 75.78 | 7 |
| 20 | ATOM | 104 | C | LYS | A | 223 | 31.913 | 18.565 | 39.681 | 1.00 | 42.81 | 6 |
| | ATOM | 105 | O | LYS | A | 223 | 30.936 | 18.323 | 38.984 | 1.00 | 40.36 | 8 |
| | ATOM | 106 | N | THR | A | 224 | 31.849 | 19.236 | 40.833 | 1.00 | 39.89 | 7 |
| | ATOM | 107 | CA | THR | A | 224 | 30.602 | 19.792 | 41.378 | 1.00 | 39.93 | 6 |
| | ATOM | 108 | CB | THR | A | 224 | 30.805 | 20.206 | 42.851 | 1.00 | 40.57 | 6 |
| 25 | ATOM | 109 | OG1 | THR | A | 224 | 31.330 | 19.113 | 43.616 | 1.00 | 39.27 | 8 |
| | ATOM | 110 | CG2 | THR | A | 224 | 29.500 | 20.684 | 43.461 | 1.00 | 38.11 | 6 |
| | ATOM | 111 | C | THR | A | 224 | 30.167 | 21.011 | 40.533 | 1.00 | 39.96 | 6 |
| | ATOM | 112 | O | THR | A | 224 | 29.313 | 20.899 | 39.655 | 1.00 | 36.67 | 8 |
| | ATOM | 113 | N | VAL | A | 225 | 30.777 | 22.160 | 40.832 | 1.00 | 38.02 | 7 |
| 30 | ATOM | 114 | CA | VAL | A | 225 | 30.532 | 23.426 | 40.137 | 1.00 | 38.12 | 6 |
| | ATOM | 115 | CB | VAL | A | 225 | 31.797 | 24.292 | 40.122 | 1.00 | 38.19 | 6 |
| | ATOM | 116 | CG1 | VAL | A | 225 | 31.512 | 25.636 | 39.491 | 1.00 | 36.77 | 6 |
| | ATOM | 117 | CG2 | VAL | A | 225 | 32.343 | 24.464 | 41.505 | 1.00 | 41.76 | 6 |
| | ATOM | 118 | C | VAL | A | 225 | 30.070 | 23.195 | 38.706 | 1.00 | 37.52 | 6 |
| 35 | ATOM | 119 | O | VAL | A | 225 | 29.119 | 23.803 | 38.239 | 1.00 | 36.77 | 8 |
| | ATOM | 120 | N | THR | A | 226 | 30.783 | 22.316 | 38.018 | 1.00 | 34.02 | 7 |
| | ATOM | 121 | CA | THR | A | 226 | 30.489 | 21.971 | 36.636 | 1.00 | 34.67 | 6 |
| | ATOM | 122 | CB | THR | A | 226 | 31.565 | 20.999 | 36.083 | 1.00 | 30.56 | 6 |
| | ATOM | 123 | OG1 | THR | A | 226 | 32.805 | 21.696 | 35.889 | 1.00 | 32.20 | 8 |
| 40 | ATOM | 124 | CG2 | THR | A | 226 | 31.108 | 20.346 | 34.783 | 1.00 | 20.99 | 6 |
| | ATOM | 125 | C | THR | A | 226 | 29.100 | 21.361 | 36.510 | 1.00 | 36.41 | 6 |
| | ATOM | 126 | O | THR | A | 226 | 28.255 | 21.877 | 35.785 | 1.00 | 39.64 | 8 |
| | ATOM | 127 | N | ALA | A | 227 | 28.880 | 20.260 | 37.222 | 1.00 | 39.20 | 7 |
| | ATOM | 128 | CA | ALA | A | 227 | 27.602 | 19.562 | 37.204 | 1.00 | 36.93 | 6 |
| 45 | ATOM | 129 | CB | ALA | A | 227 | 27.526 | 18.600 | 38.381 | 1.00 | 38.06 | 6 |
| | ATOM | 130 | C | ALA | A | 227 | 26.507 | 20.604 | 37.318 | 1.00 | 37.69 | 6 |
| | ATOM | 131 | O | ALA | A | 227 | 25.444 | 20.489 | 36.718 | 1.00 | 40.94 | 8 |
| | ATOM | 132 | N | ALA | A | 228 | 26.811 | 21.630 | 38.107 | 1.00 | 32.86 | 7 |
| | ATOM | 133 | CA | ALA | A | 228 | 25.903 | 22.734 | 38.356 | 1.00 | 32.48 | 6 |
| 50 | ATOM | 134 | CB | ALA | A | 228 | 26.448 | 23.587 | 39.486 | 1.00 | 28.25 | 6 |
| | ATOM | 135 | C | ALA | A | 228 | 25.732 | 23.570 | 37.101 | 1.00 | 36.12 | 6 |
| | ATOM | 136 | O | ALA | A | 228 | 24.673 | 23.560 | 36.473 | 1.00 | 37.86 | 8 |
| | ATOM | 137 | N | HIS | A | 229 | 26.782 | 24.306 | 36.752 | 1.00 | 33.58 | 7 |
| | ATOM | 138 | CA | HIS | A | 229 | 26.762 | 25.158 | 35.585 | 1.00 | 32.97 | 6 |
| 55 | ATOM | 139 | CB | HIS | A | 229 | 28.155 | 25.691 | 35.266 | 1.00 | 33.69 | 6 |
| | ATOM | 140 | CG | HIS | A | 229 | 28.250 | 26.333 | 33.929 | 1.00 | 28.39 | 6 |
| | ATOM | 141 | CD2 | HIS | A | 229 | 29.025 | 26.081 | 32.838 | 1.00 | 28.83 | 6 |
| | ATOM | 142 | ND1 | HIS | A | 229 | 27.386 | 27.368 | 33.542 | 1.00 | 30.47 | 7 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 143 | CE1 | HIS | A | 229 | 27.654 | 27.692 | 32.280 | 1.00 | 26.95 | 6 |
| | ATOM | 144 | NE2 | HIS | A | 229 | 28.635 | 26.934 | 31.840 | 1.00 | 31.27 | 7 |
| | ATOM | 145 | C | HIS | A | 229 | 26.225 | 24.541 | 34.312 | 1.00 | 38.40 | 6 |
| | ATOM | 146 | O | HIS | A | 229 | 25.591 | 25.227 | 33.528 | 1.00 | 41.49 | 8 |
| | ATOM | 147 | N | VAL | A | 230 | 26.519 | 23.256 | 34.113 | 1.00 | 38.55 | 7 |
| 10 | ATOM | 148 | CA | VAL | A | 230 | 26.088 | 22.554 | 32.916 | 1.00 | 40.40 | 6 |
| | ATOM | 149 | CB | VAL | A | 230 | 26.890 | 21.256 | 32.701 | 1.00 | 44.68 | 6 |
| | ATOM | 150 | CG1 | VAL | A | 230 | 26.557 | 20.656 | 31.345 | 1.00 | 39.39 | 6 |
| | ATOM | 151 | CG2 | VAL | A | 230 | 28.381 | 21.509 | 32.817 | 1.00 | 42.18 | 6 |
| | ATOM | 152 | C | VAL | A | 230 | 24.603 | 22.239 | 32.900 | 1.00 | 44.28 | 6 |
| 15 | ATOM | 153 | O | VAL | A | 230 | 23.959 | 22.316 | 31.847 | 1.00 | 45.94 | 8 |
| | ATOM | 154 | N | ALA | A | 231 | 24.072 | 21.862 | 34.059 | 1.00 | 45.59 | 7 |
| | ATOM | 155 | CA | ALA | A | 231 | 22.669 | 21.500 | 34.175 | 1.00 | 47.84 | 6 |
| | ATOM | 156 | CB | ALA | A | 231 | 22.482 | 20.582 | 35.374 | 1.00 | 45.08 | 6 |
| | ATOM | 157 | C | ALA | A | 231 | 21.792 | 22.734 | 34.314 | 1.00 | 48.04 | 6 |
| 20 | ATOM | 158 | O | ALA | A | 231 | 20.565 | 22.647 | 34.324 | 1.00 | 49.95 | 8 |
| | ATOM | 159 | N | THR | A | 232 | 22.436 | 23.894 | 34.384 | 1.00 | 47.26 | 7 |
| | ATOM | 160 | CA | THR | A | 232 | 21.722 | 25.161 | 34.528 | 1.00 | 43.64 | 6 |
| | ATOM | 161 | CB | THR | A | 232 | 22.112 | 25.832 | 35.850 | 1.00 | 41.93 | 6 |
| | ATOM | 162 | OG1 | THR | A | 232 | 23.467 | 26.283 | 35.791 | 1.00 | 39.10 | 8 |
| 25 | ATOM | 163 | CG2 | THR | A | 232 | 21.990 | 24.846 | 37.008 | 1.00 | 29.80 | 6 |
| | ATOM | 164 | C | THR | A | 232 | 22.055 | 26.114 | 33.387 | 1.00 | 43.97 | 6 |
| | ATOM | 165 | O | THR | A | 232 | 21.679 | 27.279 | 33.436 | 1.00 | 40.55 | 8 |
| | ATOM | 166 | N | ASN | A | 233 | 22.783 | 25.625 | 32.381 | 1.00 | 48.62 | 7 |
| | ATOM | 167 | CA | ASN | A | 233 | 23.134 | 26.468 | 31.231 | 1.00 | 58.62 | 6 |
| 30 | ATOM | 168 | CB | ASN | A | 233 | 24.626 | 26.283 | 30.880 | 1.00 | 62.44 | 6 |
| | ATOM | 169 | CG | ASN | A | 233 | 25.141 | 27.355 | 29.927 | 1.00 | 68.35 | 6 |
| | ATOM | 170 | OD1 | ASN | A | 233 | 24.822 | 28.544 | 30.096 | 1.00 | 65.50 | 8 |
| | ATOM | 171 | ND2 | ASN | A | 233 | 25.951 | 26.951 | 28.959 | 1.00 | 74.29 | 7 |
| | ATOM | 172 | C | ASN | A | 233 | 22.241 | 26.035 | 30.073 | 1.00 | 65.06 | 6 |
| 35 | ATOM | 173 | O | ASN | A | 233 | 22.312 | 24.900 | 29.604 | 1.00 | 69.47 | 8 |
| | ATOM | 174 | N | ALA | A | 234 | 21.381 | 26.954 | 29.646 | 1.00 | 68.80 | 7 |
| | ATOM | 175 | CA | ALA | A | 234 | 20.423 | 26.708 | 28.564 | 1.00 | 70.98 | 6 |
| | ATOM | 176 | CB | ALA | A | 234 | 19.748 | 28.015 | 28.186 | 1.00 | 71.43 | 6 |
| | ATOM | 177 | C | ALA | A | 234 | 20.988 | 26.062 | 27.308 | 1.00 | 73.83 | 6 |
| 40 | ATOM | 178 | O | ALA | A | 234 | 22.041 | 26.419 | 26.822 | 1.00 | 74.33 | 8 |
| | ATOM | 179 | N | GLN | A | 235 | 20.227 | 25.096 | 26.819 | 1.00 | 75.07 | 7 |
| | ATOM | 180 | CA | GLN | A | 235 | 20.562 | 24.363 | 25.629 | 1.00 | 76.32 | 6 |
| | ATOM | 181 | CB | GLN | A | 235 | 20.328 | 25.239 | 24.391 | 1.00 | 76.98 | 6 |
| | ATOM | 182 | CG | GLN | A | 235 | 18.887 | 25.292 | 23.908 | 1.00 | 77.07 | 6 |
| 45 | ATOM | 183 | CD | GLN | A | 235 | 17.896 | 25.420 | 25.019 | 1.00 | 80.85 | 6 |
| | ATOM | 184 | OE1 | GLN | A | 235 | 17.668 | 24.448 | 25.768 | 1.00 | 82.01 | 8 |
| | ATOM | 185 | NE2 | GLN | A | 235 | 17.313 | 26.596 | 25.149 | 1.00 | 78.80 | 7 |
| | ATOM | 186 | C | GLN | A | 235 | 21.960 | 23.840 | 25.573 | 1.00 | 77.15 | 6 |
| | ATOM | 187 | O | GLN | A | 235 | 22.386 | 23.458 | 24.508 | 1.00 | 76.06 | 8 |
| 50 | ATOM | 188 | N | GLY | A | 236 | 22.676 | 23.766 | 26.687 | 1.00 | 77.46 | 7 |
| | ATOM | 189 | CA | GLY | A | 236 | 24.053 | 23.245 | 26.627 | 1.00 | 78.37 | 6 |
| | ATOM | 190 | C | GLY | A | 236 | 24.923 | 23.491 | 25.390 | 1.00 | 79.43 | 6 |
| | ATOM | 191 | O | GLY | A | 236 | 24.917 | 24.565 | 24.844 | 1.00 | 79.47 | 8 |
| | ATOM | 192 | N | SER | A | 237 | 25.739 | 22.526 | 24.991 | 1.00 | 77.98 | 7 |
| 55 | ATOM | 193 | CA | SER | A | 237 | 26.566 | 22.760 | 23.801 | 1.00 | 76.49 | 6 |
| | ATOM | 194 | CB | SER | A | 237 | 27.981 | 22.206 | 24.015 | 1.00 | 76.46 | 6 |
| | ATOM | 195 | OG | SER | A | 237 | 28.821 | 23.145 | 24.689 | 1.00 | 40.00 | 8 |
| | ATOM | 196 | C | SER | A | 237 | 25.938 | 22.127 | 22.542 | 1.00 | 75.35 | 6 |

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|----|------|-----|-----|-----------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 197 | O | SER A 237 | 26.605 | 21.418 | 21.797 | 1.00 | 75.47 | 8 |
| | ATOM | 198 | N | HIS A 238 | 24.648 | 22.410 | 22.353 | 1.00 | 75.56 | 7 |
| | ATOM | 199 | CA | HIS A 238 | 23.842 | 21.981 | 21.236 | 1.00 | 75.46 | 6 |
| | ATOM | 200 | CB | HIS A 238 | 22.990 | 20.732 | 21.661 | 1.00 | 75.85 | 6 |
| | ATOM | 201 | CG | HIS A 238 | 22.408 | 19.933 | 20.542 | 1.00 | 40.00 | 6 |
| 10 | ATOM | 202 | CD2 | HIS A 238 | 22.790 | 18.757 | 19.957 | 1.00 | 40.00 | 6 |
| | ATOM | 203 | ND1 | HIS A 238 | 21.223 | 20.303 | 19.875 | 1.00 | 40.00 | 7 |
| | ATOM | 204 | CE1 | HIS A 238 | 20.951 | 19.365 | 18.953 | 1.00 | 40.00 | 6 |
| | ATOM | 205 | NE2 | HIS A 238 | 21.874 | 18.444 | 18.994 | 1.00 | 40.00 | 7 |
| | ATOM | 206 | C | HIS A 238 | 22.971 | 23.284 | 20.964 | 1.00 | 74.10 | 6 |
| 15 | ATOM | 207 | O | HIS A 238 | 21.863 | 23.137 | 20.441 | 1.00 | 75.34 | 8 |
| | ATOM | 208 | N | TRP A 239 | 23.487 | 24.510 | 21.368 | 1.00 | 73.39 | 7 |
| | ATOM | 209 | CA | TRP A 239 | 22.872 | 25.894 | 21.195 | 1.00 | 74.02 | 6 |
| | ATOM | 210 | CB | TRP A 239 | 23.563 | 27.026 | 22.005 | 1.00 | 81.77 | 6 |
| | ATOM | 211 | CG | TRP A 239 | 25.022 | 27.366 | 21.688 | 1.00 | 89.67 | 6 |
| 20 | ATOM | 212 | CD2 | TRP A 239 | 25.532 | 28.662 | 21.240 | 1.00 | 93.19 | 6 |
| | ATOM | 213 | CE2 | TRP A 239 | 26.961 | 28.522 | 21.136 | 1.00 | 95.46 | 6 |
| | ATOM | 214 | CE3 | TRP A 239 | 24.936 | 29.911 | 20.969 | 1.00 | 95.35 | 6 |
| | ATOM | 215 | CD1 | TRP A 239 | 26.102 | 26.548 | 21.781 | 1.00 | 94.16 | 6 |
| | ATOM | 216 | NE1 | TRP A 239 | 27.268 | 27.241 | 21.475 | 1.00 | 97.48 | 7 |
| 25 | ATOM | 217 | CZ2 | TRP A 239 | 27.798 | 29.598 | 20.764 | 1.00 | 96.23 | 6 |
| | ATOM | 218 | CZ3 | TRP A 239 | 25.763 | 30.967 | 20.569 | 1.00 | 96.75 | 6 |
| | ATOM | 219 | CH2 | TRP A 239 | 27.171 | 30.825 | 20.482 | 1.00 | 97.32 | 6 |
| | ATOM | 220 | C | TRP A 239 | 22.799 | 26.407 | 19.774 | 1.00 | 70.77 | 6 |
| | ATOM | 221 | O | TRP A 239 | 21.706 | 26.562 | 19.263 | 1.00 | 71.70 | 8 |
| 30 | ATOM | 222 | N | LYS A 240 | 23.946 | 26.701 | 19.157 | 1.00 | 67.10 | 7 |
| | ATOM | 223 | CA | LYS A 240 | 23.978 | 27.180 | 17.783 | 1.00 | 65.63 | 6 |
| | ATOM | 224 | CB | LYS A 240 | 25.314 | 26.780 | 17.153 | 1.00 | 66.65 | 6 |
| | ATOM | 225 | CG | LYS A 240 | 26.529 | 27.342 | 17.872 | 1.00 | 69.83 | 6 |
| | ATOM | 226 | CD | LYS A 240 | 27.805 | 27.037 | 17.108 | 1.00 | 71.49 | 6 |
| 35 | ATOM | 227 | CE | LYS A 240 | 28.980 | 27.720 | 17.776 | 1.00 | 71.31 | 6 |
| | ATOM | 228 | NZ | LYS A 240 | 30.238 | 27.438 | 17.034 | 1.00 | 72.23 | 7 |
| | ATOM | 229 | C | LYS A 240 | 22.808 | 26.699 | 16.895 | 1.00 | 66.19 | 6 |
| | ATOM | 230 | O | LYS A 240 | 22.550 | 27.298 | 15.851 | 1.00 | 65.20 | 8 |
| | ATOM | 231 | N | ASN A 241 | 22.113 | 25.640 | 17.325 | 1.00 | 66.69 | 7 |
| 40 | ATOM | 232 | CA | ASN A 241 | 20.976 | 25.078 | 16.599 | 1.00 | 67.53 | 6 |
| | ATOM | 233 | CB | ASN A 241 | 21.122 | 23.562 | 16.550 | 1.00 | 67.98 | 6 |
| | ATOM | 234 | CG | ASN A 241 | 22.304 | 23.121 | 15.693 | 1.00 | 70.19 | 6 |
| | ATOM | 235 | OD1 | ASN A 241 | 22.404 | 23.506 | 14.503 | 1.00 | 71.37 | 8 |
| | ATOM | 236 | ND2 | ASN A 241 | 23.176 | 22.310 | 16.271 | 1.00 | 71.48 | 7 |
| 45 | ATOM | 237 | C | ASN A 241 | 19.570 | 25.421 | 17.152 | 1.00 | 66.62 | 6 |
| | ATOM | 238 | O | ASN A 241 | 18.581 | 24.822 | 16.731 | 1.00 | 64.76 | 8 |
| | ATOM | 239 | N | LYS A 242 | 19.475 | 26.380 | 18.069 | 1.00 | 66.86 | 7 |
| | ATOM | 240 | CA | LYS A 242 | 18.191 | 26.786 | 18.642 | 1.00 | 67.46 | 6 |
| | ATOM | 241 | CB | LYS A 242 | 18.164 | 26.396 | 20.119 | 1.00 | 67.93 | 6 |
| 50 | ATOM | 242 | CG | LYS A 242 | 18.250 | 24.896 | 20.337 | 1.00 | 71.52 | 6 |
| | ATOM | 243 | CD | LYS A 242 | 17.004 | 24.149 | 19.821 | 1.00 | 74.32 | 6 |
| | ATOM | 244 | CE | LYS A 242 | 15.755 | 24.491 | 20.643 | 1.00 | 74.41 | 6 |
| | ATOM | 245 | NZ | LYS A 242 | 15.927 | 24.161 | 22.109 | 1.00 | 74.44 | 7 |
| | ATOM | 246 | C | LYS A 242 | 18.143 | 28.291 | 18.483 | 1.00 | 66.28 | 6 |
| 55 | ATOM | 247 | O | LYS A 242 | 17.102 | 28.923 | 18.592 | 1.00 | 67.61 | 8 |
| | ATOM | 248 | N | ARG A 243 | 19.334 | 28.813 | 18.204 | 1.00 | 64.19 | 7 |
| | ATOM | 249 | CA | ARG A 243 | 19.617 | 30.219 | 17.975 | 1.00 | 62.43 | 6 |
| | ATOM | 250 | CB | ARG A 243 | 21.070 | 30.274 | 17.463 | 1.00 | 60.12 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 251 | CG | ARG | A | 243 | 21.665 | 31.636 | 17.305 | 1.00 | 40.00 | 6 |
| | ATOM | 252 | CD | ARG | A | 243 | 23.213 | 31.599 | 17.267 | 1.00 | 40.00 | 6 |
| | ATOM | 253 | NE | ARG | A | 243 | 23.826 | 31.217 | 15.996 | 1.00 | 40.00 | 7 |
| | ATOM | 254 | CZ | ARG | A | 243 | 25.113 | 31.439 | 15.714 | 1.00 | 40.00 | 6 |
| | ATOM | 255 | NH1 | ARG | A | 243 | 25.905 | 32.041 | 16.616 | 1.00 | 40.00 | 7 |
| 10 | ATOM | 256 | NH2 | ARG | A | 243 | 25.592 | 31.097 | 14.520 | 1.00 | 40.00 | 7 |
| | ATOM | 257 | C | ARG | A | 243 | 18.639 | 30.789 | 16.950 | 1.00 | 62.97 | 6 |
| | ATOM | 258 | O | ARG | A | 243 | 18.662 | 30.390 | 15.784 | 1.00 | 63.96 | 8 |
| | ATOM | 259 | N | LYS | A | 244 | 17.771 | 31.692 | 17.393 | 1.00 | 62.41 | 7 |
| | ATOM | 260 | CA | LYS | A | 244 | 16.790 | 32.309 | 16.498 | 1.00 | 61.57 | 6 |
| 15 | ATOM | 261 | CB | LYS | A | 244 | 15.368 | 31.974 | 16.962 | 1.00 | 63.68 | 6 |
| | ATOM | 262 | CG | LYS | A | 244 | 15.102 | 30.471 | 17.104 | 1.00 | 71.29 | 6 |
| | ATOM | 263 | CD | LYS | A | 244 | 13.641 | 30.167 | 17.468 | 1.00 | 73.83 | 6 |
| | ATOM | 264 | CE | LYS | A | 244 | 13.182 | 30.908 | 18.737 | 1.00 | 74.71 | 6 |
| | ATOM | 265 | NZ | LYS | A | 244 | 13.951 | 30.536 | 19.970 | 1.00 | 73.32 | 7 |
| 20 | ATOM | 266 | C | LYS | A | 244 | 17.009 | 33.806 | 16.501 | 1.00 | 59.30 | 6 |
| | ATOM | 267 | O | LYS | A | 244 | 16.562 | 34.514 | 17.399 | 1.00 | 56.34 | 8 |
| | ATOM | 268 | N | PHE | A | 245 | 17.705 | 34.264 | 15.468 | 1.00 | 57.06 | 7 |
| | ATOM | 269 | CA | PHE | A | 245 | 18.045 | 35.692 | 15.333 | 1.00 | 59.01 | 6 |
| | ATOM | 270 | CB | PHE | A | 245 | 18.825 | 35.947 | 14.049 | 1.00 | 59.62 | 6 |
| 25 | ATOM | 271 | CG | PHE | A | 245 | 19.908 | 34.979 | 13.834 | 1.00 | 66.60 | 6 |
| | ATOM | 272 | CD1 | PHE | A | 245 | 19.618 | 33.714 | 13.399 | 1.00 | 67.17 | 6 |
| | ATOM | 273 | CD2 | PHE | A | 245 | 21.198 | 35.309 | 14.139 | 1.00 | 69.25 | 6 |
| | ATOM | 274 | CE1 | PHE | A | 245 | 20.614 | 32.794 | 13.255 | 1.00 | 69.92 | 6 |
| | ATOM | 275 | CE2 | PHE | A | 245 | 22.189 | 34.385 | 13.994 | 1.00 | 70.50 | 6 |
| 30 | ATOM | 276 | CZ | PHE | A | 245 | 21.897 | 33.126 | 13.552 | 1.00 | 70.89 | 6 |
| | ATOM | 277 | C | PHE | A | 245 | 16.856 | 36.620 | 15.340 | 1.00 | 60.68 | 6 |
| | ATOM | 278 | O | PHE | A | 245 | 15.946 | 36.516 | 14.528 | 1.00 | 62.37 | 8 |
| | ATOM | 279 | N | LEU | A | 246 | 16.919 | 37.558 | 16.272 | 1.00 | 60.10 | 7 |
| | ATOM | 280 | CA | LEU | A | 246 | 15.884 | 38.554 | 16.437 | 1.00 | 59.44 | 6 |
| 35 | ATOM | 281 | CB | LEU | A | 246 | 16.227 | 39.510 | 17.585 | 1.00 | 57.43 | 6 |
| | ATOM | 282 | CG | LEU | A | 246 | 15.100 | 40.384 | 18.086 | 1.00 | 54.41 | 6 |
| | ATOM | 283 | CD1 | LEU | A | 246 | 14.010 | 39.474 | 18.640 | 1.00 | 52.43 | 6 |
| | ATOM | 284 | CD2 | LEU | A | 246 | 15.575 | 41.325 | 19.151 | 1.00 | 51.69 | 6 |
| | ATOM | 285 | C | LEU | A | 246 | 15.717 | 39.330 | 15.135 | 1.00 | 62.05 | 6 |
| 40 | ATOM | 286 | O | LEU | A | 246 | 16.706 | 39.609 | 14.430 | 1.00 | 59.85 | 8 |
| | ATOM | 287 | N | PRO | A | 247 | 14.473 | 39.668 | 14.784 | 1.00 | 63.33 | 7 |
| | ATOM | 288 | CD | PRO | A | 247 | 13.263 | 39.314 | 15.534 | 1.00 | 64.44 | 6 |
| | ATOM | 289 | CA | PRO | A | 247 | 14.198 | 40.421 | 13.558 | 1.00 | 63.56 | 6 |
| | ATOM | 290 | CB | PRO | A | 247 | 12.687 | 40.671 | 13.600 | 1.00 | 64.42 | 6 |
| 45 | ATOM | 291 | CG | PRO | A | 247 | 12.161 | 39.922 | 14.729 | 1.00 | 64.90 | 6 |
| | ATOM | 292 | C | PRO | A | 247 | 14.996 | 41.733 | 13.496 | 1.00 | 61.94 | 6 |
| | ATOM | 293 | O | PRO | A | 247 | 15.159 | 42.455 | 14.486 | 1.00 | 61.60 | 8 |
| | ATOM | 294 | N | GLU | A | 248 | 15.506 | 42.006 | 12.299 | 1.00 | 61.33 | 7 |
| | ATOM | 295 | CA | GLU | A | 248 | 16.280 | 43.197 | 11.976 | 1.00 | 63.50 | 6 |
| 50 | ATOM | 296 | CB | GLU | A | 248 | 16.481 | 43.273 | 10.437 | 1.00 | 66.94 | 6 |
| | ATOM | 297 | CG | GLU | A | 248 | 17.012 | 44.671 | 9.966 | 1.00 | 68.70 | 6 |
| | ATOM | 298 | CD | GLU | A | 248 | 16.981 | 44.939 | 8.471 | 1.00 | 40.00 | 6 |
| | ATOM | 299 | OE1 | GLU | A | 248 | 16.432 | 44.144 | 7.644 | 1.00 | 40.00 | 8 |
| | ATOM | 300 | OE2 | GLU | A | 248 | 17.509 | 46.015 | 8.086 | 1.00 | 40.00 | 8 |
| 55 | ATOM | 301 | C | GLU | A | 248 | 15.624 | 44.489 | 12.458 | 1.00 | 64.19 | 6 |
| | ATOM | 302 | O | GLU | A | 248 | 16.298 | 45.395 | 12.918 | 1.00 | 65.56 | 8 |
| | ATOM | 303 | N | ASP | A | 249 | 14.300 | 44.545 | 12.323 | 1.00 | 64.36 | 7 |
| | ATOM | 304 | CA | ASP | A | 249 | 13.493 | 45.703 | 12.673 | 1.00 | 63.33 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 305 | CB | ASP | A | 249 | 12.088 | 45.531 | 12.116 | 1.00 | 62.97 | 6 |
| | ATOM | 306 | CG | ASP | A | 249 | 11.277 | 44.527 | 12.870 | 1.00 | 64.63 | 6 |
| | ATOM | 307 | OD1 | ASP | A | 249 | 11.687 | 43.352 | 12.963 | 1.00 | 64.84 | 8 |
| | ATOM | 308 | OD2 | ASP | A | 249 | 10.183 | 44.880 | 13.395 | 1.00 | 66.52 | 8 |
| | ATOM | 309 | C | ASP | A | 249 | 13.371 | 46.062 | 14.130 | 1.00 | 64.31 | 6 |
| 10 | ATOM | 310 | O | ASP | A | 249 | 13.310 | 47.250 | 14.468 | 1.00 | 64.73 | 8 |
| | ATOM | 311 | N | ILE | A | 250 | 13.274 | 45.049 | 14.997 | 1.00 | 63.09 | 7 |
| | ATOM | 312 | CA | ILE | A | 250 | 13.133 | 45.318 | 16.418 | 1.00 | 64.39 | 6 |
| | ATOM | 313 | CB | ILE | A | 250 | 13.035 | 44.034 | 17.214 | 1.00 | 65.79 | 6 |
| | ATOM | 314 | CG2 | ILE | A | 250 | 12.001 | 44.104 | 18.336 | 1.00 | 64.78 | 6 |
| 15 | ATOM | 315 | CG1 | ILE | A | 250 | 12.611 | 42.860 | 16.341 | 1.00 | 65.28 | 6 |
| | ATOM | 316 | CD1 | ILE | A | 250 | 11.753 | 41.852 | 17.088 | 1.00 | 65.08 | 6 |
| | ATOM | 317 | C | ILE | A | 250 | 14.404 | 46.104 | 17.276 | 1.00 | 65.21 | 6 |
| | ATOM | 318 | O | ILE | A | 250 | 15.155 | 45.506 | 18.047 | 1.00 | 64.05 | 8 |
| | ATOM | 319 | N | GLY | A | 251 | 14.670 | 47.529 | 17.299 | 1.00 | 65.48 | 7 |
| 20 | ATOM | 320 | CA | GLY | A | 251 | 15.871 | 48.326 | 18.042 | 1.00 | 67.32 | 6 |
| | ATOM | 321 | C | GLY | A | 251 | 16.595 | 49.110 | 16.895 | 1.00 | 68.52 | 6 |
| | ATOM | 322 | O | GLY | A | 251 | 17.528 | 48.616 | 16.266 | 1.00 | 65.49 | 8 |
| | ATOM | 323 | N | GLN | A | 252 | 16.162 | 50.356 | 16.557 | 1.00 | 72.26 | 7 |
| | ATOM | 324 | CA | GLN | A | 252 | 16.541 | 50.930 | 15.207 | 1.00 | 74.10 | 6 |
| 25 | ATOM | 325 | CB | GLN | A | 252 | 15.316 | 50.844 | 14.295 | 1.00 | 75.82 | 6 |
| | ATOM | 326 | C | GLN | A | 252 | 16.995 | 52.403 | 15.084 | 1.00 | 77.17 | 6 |
| | ATOM | 327 | O | GLN | A | 252 | 17.572 | 52.955 | 15.986 | 1.00 | 76.50 | 8 |
| | ATOM | 328 | N | ALA | A | 253 | 16.374 | 53.372 | 13.908 | 1.00 | 80.78 | 7 |
| | ATOM | 329 | CA | ALA | A | 253 | 16.687 | 54.725 | 13.567 | 1.00 | 83.70 | 6 |
| 30 | ATOM | 330 | CB | ALA | A | 253 | 16.381 | 54.956 | 12.093 | 1.00 | 83.23 | 6 |
| | ATOM | 331 | C | ALA | A | 253 | 16.159 | 55.960 | 14.345 | 1.00 | 85.59 | 6 |
| | ATOM | 332 | O | ALA | A | 253 | 15.317 | 56.721 | 13.798 | 1.00 | 85.69 | 8 |
| | ATOM | 333 | N | PRO | A | 254 | 16.384 | 56.155 | 16.264 | 1.00 | 35.05 | 7 |
| | ATOM | 334 | CD | PRO | A | 254 | 17.102 | 55.053 | 16.908 | 1.00 | 33.97 | 6 |
| 35 | ATOM | 335 | CA | PRO | A | 254 | 16.002 | 57.231 | 17.219 | 1.00 | 35.89 | 6 |
| | ATOM | 336 | CB | PRO | A | 254 | 16.534 | 56.756 | 18.563 | 1.00 | 33.94 | 6 |
| | ATOM | 337 | CG | PRO | A | 254 | 17.146 | 55.441 | 18.349 | 1.00 | 33.31 | 6 |
| | ATOM | 338 | C | PRO | A | 254 | 16.717 | 58.498 | 16.731 | 1.00 | 37.75 | 6 |
| | ATOM | 339 | O | PRO | A | 254 | 17.838 | 58.804 | 17.100 | 1.00 | 38.78 | 8 |
| 40 | TER | | | | | | | | | | | |
| | ATOM | 1 | N | LYS | A | 263 | 18.045 | 57.462 | 23.875 | 1.00 | 61.71 | 7 |
| | ATOM | 2 | CA | LYS | A | 263 | 16.824 | 56.712 | 24.215 | 1.00 | 64.36 | 6 |
| | ATOM | 3 | CB | LYS | A | 263 | 15.758 | 57.004 | 23.141 | 1.00 | 63.50 | 6 |
| | ATOM | 4 | C | LYS | A | 263 | 16.841 | 55.180 | 24.429 | 1.00 | 63.41 | 6 |
| 45 | ATOM | 5 | O | LYS | A | 263 | 17.877 | 54.542 | 24.409 | 1.00 | 61.93 | 8 |
| | ATOM | 6 | N | VAL | A | 264 | 15.615 | 54.664 | 24.654 | 1.00 | 61.15 | 7 |
| | ATOM | 7 | CA | VAL | A | 264 | 15.292 | 53.229 | 24.856 | 1.00 | 59.46 | 6 |
| | ATOM | 8 | CB | VAL | A | 264 | 14.251 | 52.974 | 25.978 | 1.00 | 59.03 | 6 |
| | ATOM | 9 | CG1 | VAL | A | 264 | 14.229 | 51.494 | 26.368 | 1.00 | 53.79 | 6 |
| 50 | ATOM | 10 | CG2 | VAL | A | 264 | 14.449 | 53.818 | 27.142 | 1.00 | 55.32 | 6 |
| | ATOM | 11 | C | VAL | A | 264 | 14.590 | 52.820 | 23.554 | 1.00 | 60.96 | 6 |
| | ATOM | 12 | O | VAL | A | 264 | 14.734 | 53.468 | 22.508 | 1.00 | 62.13 | 8 |
| | ATOM | 13 | N | ASP | A | 265 | 13.802 | 51.755 | 23.634 | 1.00 | 62.59 | 7 |
| | ATOM | 14 | CA | ASP | A | 265 | 12.995 | 51.263 | 22.526 | 1.00 | 64.95 | 6 |
| 55 | ATOM | 15 | CB | ASP | A | 265 | 13.825 | 51.077 | 21.271 | 1.00 | 64.32 | 6 |
| | ATOM | 16 | CG | ASP | A | 265 | 13.282 | 50.048 | 20.485 | 1.00 | 67.70 | 6 |
| | ATOM | 17 | OD1 | ASP | A | 265 | 12.795 | 50.011 | 19.446 | 1.00 | 72.59 | 8 |
| | ATOM | 18 | OD2 | ASP | A | 265 | 13.354 | 48.867 | 20.294 | 1.00 | 68.84 | 8 |

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|----|------|----|-----|-----------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 19 | C | ASP A 265 | 12.326 | 49.943 | 22.952 | 1.00 | 65.64 | 6 |
| | ATOM | 20 | O | ASP A 265 | 12.771 | 48.850 | 22.655 | 1.00 | 68.81 | 8 |
| | ATOM | 21 | N | LEU A 266 | 11.256 | 50.152 | 23.702 | 1.00 | 65.12 | 7 |
| | ATOM | 22 | CA | LEU A 266 | 10.368 | 49.169 | 24.288 | 1.00 | 63.40 | 6 |
| | ATOM | 23 | CB | LEU A 266 | 9.115 | 49.938 | 24.708 | 1.00 | 67.34 | 6 |
| 10 | ATOM | 24 | CG | LEU A 266 | 9.399 | 51.124 | 25.618 | 1.00 | 69.35 | 6 |
| | ATOM | 25 | CD1 | LEU A 266 | 8.304 | 52.148 | 25.533 | 1.00 | 68.24 | 6 |
| | ATOM | 26 | CD2 | LEU A 266 | 9.581 | 50.631 | 27.021 | 1.00 | 70.47 | 6 |
| | ATOM | 27 | C | LEU A 266 | 9.940 | 47.888 | 23.559 | 1.00 | 59.67 | 6 |
| | ATOM | 28 | O | LEU A 266 | 9.694 | 46.879 | 24.220 | 1.00 | 53.35 | 8 |
| 15 | ATOM | 29 | N | GLU A 267 | 9.815 | 47.904 | 22.235 | 1.00 | 58.01 | 7 |
| | ATOM | 30 | CA | GLU A 267 | 9.417 | 46.682 | 21.572 | 1.00 | 58.34 | 6 |
| | ATOM | 31 | CB | GLU A 267 | 9.311 | 46.855 | 20.048 | 1.00 | 59.21 | 6 |
| | ATOM | 32 | CG | GLU A 267 | 9.129 | 45.494 | 19.322 | 1.00 | 62.89 | 6 |
| | ATOM | 33 | CD | GLU A 267 | 8.736 | 45.592 | 17.883 | 1.00 | 67.66 | 6 |
| 20 | ATOM | 34 | OE1 | GLU A 267 | 9.433 | 46.263 | 17.080 | 1.00 | 69.95 | 8 |
| | ATOM | 35 | OE2 | GLU A 267 | 7.710 | 44.974 | 17.503 | 1.00 | 69.40 | 8 |
| | ATOM | 36 | C | GLU A 267 | 10.504 | 45.683 | 21.895 | 1.00 | 57.67 | 6 |
| | ATOM | 37 | O | GLU A 267 | 10.255 | 44.485 | 21.988 | 1.00 | 58.34 | 8 |
| | ATOM | 38 | N | ALA A 268 | 11.712 | 46.222 | 22.054 | 1.00 | 53.43 | 7 |
| 25 | ATOM | 39 | CA | ALA A 268 | 12.903 | 45.454 | 22.374 | 1.00 | 49.00 | 6 |
| | ATOM | 40 | CB | ALA A 268 | 14.137 | 46.241 | 21.983 | 1.00 | 45.72 | 6 |
| | ATOM | 41 | C | ALA A 268 | 12.908 | 45.196 | 23.873 | 1.00 | 45.76 | 6 |
| | ATOM | 42 | O | ALA A 268 | 12.887 | 44.042 | 24.307 | 1.00 | 41.50 | 8 |
| | ATOM | 43 | N | PHE A 269 | 12.918 | 46.277 | 24.663 | 1.00 | 41.43 | 7 |
| 30 | ATOM | 44 | CA | PHE A 269 | 12.920 | 46.158 | 26.118 | 1.00 | 43.96 | 6 |
| | ATOM | 45 | CB | PHE A 269 | 12.395 | 47.426 | 26.777 | 1.00 | 40.10 | 6 |
| | ATOM | 46 | CG | PHE A 269 | 12.332 | 47.345 | 28.271 | 1.00 | 40.44 | 6 |
| | ATOM | 47 | CD1 | PHE A 269 | 13.457 | 47.595 | 29.034 | 1.00 | 38.98 | 6 |
| | ATOM | 48 | CD2 | PHE A 269 | 11.165 | 46.946 | 28.903 | 1.00 | 37.15 | 6 |
| 35 | ATOM | 49 | CE1 | PHE A 269 | 13.409 | 47.469 | 30.436 | 1.00 | 32.12 | 6 |
| | ATOM | 50 | CE2 | PHE A 269 | 11.105 | 46.815 | 30.303 | 1.00 | 38.41 | 6 |
| | ATOM | 51 | CZ | PHE A 269 | 12.228 | 47.070 | 31.071 | 1.00 | 40.55 | 6 |
| | ATOM | 52 | C | PHE A 269 | 12.017 | 45.012 | 26.520 | 1.00 | 49.76 | 6 |
| | ATOM | 53 | O | PHE A 269 | 12.277 | 44.324 | 27.484 | 1.00 | 52.15 | 8 |
| 40 | ATOM | 54 | N | SER A 270 | 10.934 | 44.835 | 25.768 | 1.00 | 53.15 | 7 |
| | ATOM | 55 | CA | SER A 270 | 9.988 | 43.768 | 26.043 | 1.00 | 52.29 | 6 |
| | ATOM | 56 | CB | SER A 270 | 8.727 | 43.943 | 25.215 | 1.00 | 51.85 | 6 |
| | ATOM | 57 | OG | SER A 270 | 7.785 | 42.918 | 25.497 | 1.00 | 53.42 | 8 |
| | ATOM | 58 | C | SER A 270 | 10.637 | 42.464 | 25.685 | 1.00 | 49.38 | 6 |
| 45 | ATOM | 59 | O | SER A 270 | 11.068 | 41.741 | 26.562 | 1.00 | 48.74 | 8 |
| | ATOM | 60 | N | HIS A 271 | 10.683 | 42.173 | 24.383 | 1.00 | 50.15 | 7 |
| | ATOM | 61 | CA | HIS A 271 | 11.276 | 40.932 | 23.877 | 1.00 | 51.67 | 6 |
| | ATOM | 62 | CB | HIS A 271 | 11.797 | 41.118 | 22.455 | 1.00 | 58.52 | 6 |
| | ATOM | 63 | CG | HIS A 271 | 10.775 | 40.885 | 21.399 | 1.00 | 68.97 | 6 |
| 50 | ATOM | 64 | CD2 | HIS A 271 | 10.633 | 39.891 | 20.485 | 1.00 | 70.88 | 6 |
| | ATOM | 65 | ND1 | HIS A 271 | 9.673 | 41.732 | 21.199 | 1.00 | 71.98 | 7 |
| | ATOM | 66 | CE1 | HIS A 271 | 8.936 | 41.242 | 20.209 | 1.00 | 73.91 | 6 |
| | ATOM | 67 | NE2 | HIS A 271 | 9.495 | 40.132 | 19.764 | 1.00 | 73.59 | 7 |
| | ATOM | 68 | C | HIS A 271 | 12.402 | 40.416 | 24.745 | 1.00 | 48.33 | 6 |
| 55 | ATOM | 69 | O | HIS A 271 | 12.707 | 39.225 | 24.728 | 1.00 | 48.39 | 8 |
| | ATOM | 70 | N | PHE A 272 | 13.029 | 41.334 | 25.487 | 1.00 | 41.34 | 7 |
| | ATOM | 71 | CA | PHE A 272 | 14.130 | 41.001 | 26.384 | 1.00 | 39.44 | 6 |
| | ATOM | 72 | CB | PHE A 272 | 15.077 | 42.194 | 26.512 | 1.00 | 36.67 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 73 | CG | PHE | A | 272 | 15.953 | 42.413 | 25.282 | 1.00 | 33.39 | 6 |
| | ATOM | 74 | CD1 | PHE | A | 272 | 16.619 | 43.615 | 25.093 | 1.00 | 33.14 | 6 |
| | ATOM | 75 | CD2 | PHE | A | 272 | 16.138 | 41.394 | 24.346 | 1.00 | 38.28 | 6 |
| | ATOM | 76 | CE1 | PHE | A | 272 | 17.454 | 43.807 | 23.988 | 1.00 | 38.26 | 6 |
| | ATOM | 77 | CE2 | PHE | A | 272 | 16.973 | 41.585 | 23.244 | 1.00 | 43.28 | 6 |
| 10 | ATOM | 78 | CZ | PHE | A | 272 | 17.634 | 42.786 | 23.068 | 1.00 | 39.74 | 6 |
| | ATOM | 79 | C | PHE | A | 272 | 13.650 | 40.528 | 27.764 | 1.00 | 40.75 | 6 |
| | ATOM | 80 | O | PHE | A | 272 | 14.081 | 39.476 | 28.227 | 1.00 | 35.51 | 8 |
| | ATOM | 81 | N | THR | A | 273 | 12.756 | 41.266 | 28.428 | 1.00 | 41.64 | 7 |
| | ATOM | 82 | CA | THR | A | 273 | 12.290 | 40.854 | 29.757 | 1.00 | 45.97 | 6 |
| 15 | ATOM | 83 | CB | THR | A | 273 | 11.651 | 42.025 | 30.506 | 1.00 | 51.52 | 6 |
| | ATOM | 84 | OG1 | THR | A | 273 | 10.442 | 42.422 | 29.859 | 1.00 | 45.74 | 8 |
| | ATOM | 85 | CG2 | THR | A | 273 | 12.601 | 43.211 | 30.565 | 1.00 | 49.73 | 6 |
| | ATOM | 86 | C | THR | A | 273 | 11.267 | 39.731 | 29.664 | 1.00 | 46.23 | 6 |
| | ATOM | 87 | O | THR | A | 273 | 10.854 | 39.183 | 30.680 | 1.00 | 41.21 | 8 |
| 20 | ATOM | 88 | N | LYS | A | 274 | 10.849 | 39.412 | 28.440 | 1.00 | 46.21 | 7 |
| | ATOM | 89 | CA | LYS | A | 274 | 9.871 | 38.362 | 28.211 | 1.00 | 54.53 | 6 |
| | ATOM | 90 | CB | LYS | A | 274 | 9.414 | 38.405 | 26.773 | 1.00 | 54.36 | 6 |
| | ATOM | 91 | C | LYS | A | 274 | 10.498 | 37.015 | 28.515 | 1.00 | 56.88 | 6 |
| | ATOM | 92 | O | LYS | A | 274 | 9.789 | 36.044 | 28.759 | 1.00 | 57.98 | 8 |
| 25 | ATOM | 93 | N | ILE | A | 275 | 11.836 | 36.973 | 28.491 | 1.00 | 56.48 | 7 |
| | ATOM | 94 | CA | ILE | A | 275 | 12.609 | 35.746 | 28.767 | 1.00 | 52.64 | 6 |
| | ATOM | 95 | CB | ILE | A | 275 | 13.444 | 35.346 | 27.543 | 1.00 | 49.15 | 6 |
| | ATOM | 96 | CG2 | ILE | A | 275 | 12.568 | 34.829 | 26.429 | 1.00 | 47.42 | 6 |
| | ATOM | 97 | CG1 | ILE | A | 275 | 14.238 | 36.532 | 27.026 | 1.00 | 45.31 | 6 |
| 30 | ATOM | 98 | CD1 | ILE | A | 275 | 15.001 | 36.242 | 25.771 | 1.00 | 37.22 | 6 |
| | ATOM | 99 | C | ILE | A | 275 | 13.541 | 35.870 | 29.982 | 1.00 | 51.78 | 6 |
| | ATOM | 100 | O | ILE | A | 275 | 14.014 | 34.873 | 30.503 | 1.00 | 49.80 | 8 |
| | ATOM | 101 | N | ILE | A | 276 | 13.790 | 37.107 | 30.415 | 1.00 | 51.76 | 7 |
| | ATOM | 102 | CA | ILE | A | 276 | 14.681 | 37.389 | 31.537 | 1.00 | 52.58 | 6 |
| 35 | ATOM | 103 | CB | ILE | A | 276 | 14.691 | 38.877 | 31.844 | 1.00 | 55.04 | 6 |
| | ATOM | 104 | CG2 | ILE | A | 276 | 13.311 | 39.340 | 32.261 | 1.00 | 53.28 | 6 |
| | ATOM | 105 | CG1 | ILE | A | 276 | 15.675 | 39.206 | 32.976 | 1.00 | 57.31 | 6 |
| | ATOM | 106 | CD1 | ILE | A | 276 | 17.096 | 38.942 | 32.655 | 1.00 | 60.32 | 6 |
| | ATOM | 107 | C | ILE | A | 276 | 14.323 | 36.644 | 32.828 | 1.00 | 50.70 | 6 |
| 40 | ATOM | 108 | O | ILE | A | 276 | 15.177 | 36.458 | 33.691 | 1.00 | 55.55 | 8 |
| | ATOM | 109 | N | THR | A | 277 | 13.072 | 36.209 | 32.963 | 1.00 | 47.33 | 7 |
| | ATOM | 110 | CA | THR | A | 277 | 12.631 | 35.523 | 34.158 | 1.00 | 42.59 | 6 |
| | ATOM | 111 | CB | THR | A | 277 | 11.098 | 35.456 | 34.217 | 1.00 | 44.97 | 6 |
| | ATOM | 112 | OG1 | THR | A | 277 | 10.545 | 36.777 | 34.102 | 1.00 | 46.38 | 8 |
| 45 | ATOM | 113 | CG2 | THR | A | 277 | 10.657 | 34.838 | 35.539 | 1.00 | 37.17 | 6 |
| | ATOM | 114 | C | THR | A | 277 | 13.211 | 34.118 | 34.304 | 1.00 | 39.84 | 6 |
| | ATOM | 115 | O | THR | A | 277 | 13.796 | 33.796 | 35.365 | 1.00 | 40.55 | 8 |
| | ATOM | 116 | N | PRO | A | 278 | 13.055 | 33.261 | 33.288 | 1.00 | 38.20 | 7 |
| | ATOM | 117 | CD | PRO | A | 278 | 12.370 | 33.534 | 32.023 | 1.00 | 36.34 | 6 |
| 50 | ATOM | 118 | CA | PRO | A | 278 | 13.595 | 31.894 | 33.363 | 1.00 | 36.63 | 6 |
| | ATOM | 119 | CB | PRO | A | 278 | 13.153 | 31.244 | 32.064 | 1.00 | 32.95 | 6 |
| | ATOM | 120 | CG | PRO | A | 278 | 12.573 | 32.291 | 31.239 | 1.00 | 35.75 | 6 |
| | ATOM | 121 | C | PRO | A | 278 | 15.101 | 31.932 | 33.476 | 1.00 | 38.60 | 6 |
| | ATOM | 122 | O | PRO | A | 278 | 15.746 | 30.981 | 33.898 | 1.00 | 37.67 | 8 |
| 55 | ATOM | 123 | N | ALA | A | 279 | 15.656 | 33.051 | 33.035 | 1.00 | 37.05 | 7 |
| | ATOM | 124 | CA | ALA | A | 279 | 17.087 | 33.277 | 33.041 | 1.00 | 33.18 | 6 |
| | ATOM | 125 | CB | ALA | A | 279 | 17.376 | 34.599 | 32.348 | 1.00 | 30.56 | 6 |
| | ATOM | 126 | C | ALA | A | 279 | 17.624 | 33.312 | 34.452 | 1.00 | 33.47 | 6 |

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|----|------|-----|-----|-----------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 127 | O | ALA A 279 | 18.523 | 32.555 | 34.789 | 1.00 | 33.74 | 8 |
| | ATOM | 128 | N | ILE A 280 | 17.060 | 34.215 | 35.260 | 1.00 | 29.96 | 7 |
| | ATOM | 129 | CA | ILE A 280 | 17.459 | 34.362 | 36.646 | 1.00 | 25.94 | 6 |
| | ATOM | 130 | CB | ILE A 280 | 16.686 | 35.484 | 37.315 | 1.00 | 26.95 | 6 |
| | ATOM | 131 | CG2 | ILE A 280 | 17.109 | 35.632 | 38.733 | 1.00 | 15.40 | 6 |
| 10 | ATOM | 132 | CG1 | ILE A 280 | 16.931 | 36.808 | 36.595 | 1.00 | 26.73 | 6 |
| | ATOM | 133 | CD1 | ILE A 280 | 16.292 | 38.002 | 37.272 | 1.00 | 34.31 | 6 |
| | ATOM | 134 | C | ILE A 280 | 17.263 | 33.066 | 37.412 | 1.00 | 31.39 | 6 |
| | ATOM | 135 | O | ILE A 280 | 18.116 | 32.679 | 38.207 | 1.00 | 35.69 | 8 |
| | ATOM | 136 | N | THR A 281 | 16.145 | 32.386 | 37.165 | 1.00 | 30.90 | 7 |
| 15 | ATOM | 137 | CA | THR A 281 | 15.854 | 31.118 | 37.851 | 1.00 | 33.49 | 6 |
| | ATOM | 138 | CB | THR A 281 | 14.598 | 30.413 | 37.277 | 1.00 | 37.18 | 6 |
| | ATOM | 139 | OG1 | THR A 281 | 14.795 | 30.099 | 35.898 | 1.00 | 46.48 | 8 |
| | ATOM | 140 | CG2 | THR A 281 | 13.352 | 31.281 | 37.444 | 1.00 | 32.85 | 6 |
| | ATOM | 141 | C | THR A 281 | 17.045 | 30.176 | 37.713 | 1.00 | 29.94 | 6 |
| 20 | ATOM | 142 | O | THR A 281 | 17.478 | 29.546 | 38.684 | 1.00 | 25.55 | 8 |
| | ATOM | 143 | N | ARG A 282 | 17.561 | 30.076 | 36.489 | 1.00 | 32.70 | 7 |
| | ATOM | 144 | CA | ARG A 282 | 18.692 | 29.198 | 36.218 | 1.00 | 34.27 | 6 |
| | ATOM | 145 | CB | ARG A 282 | 19.136 | 29.374 | 34.780 | 1.00 | 33.78 | 6 |
| | ATOM | 146 | CG | ARG A 282 | 19.272 | 28.086 | 34.013 | 1.00 | 45.15 | 6 |
| 25 | ATOM | 147 | CD | ARG A 282 | 18.179 | 27.921 | 32.977 | 1.00 | 58.24 | 6 |
| | ATOM | 148 | NE | ARG A 282 | 18.041 | 29.077 | 32.117 | 1.00 | 68.41 | 7 |
| | ATOM | 149 | CZ | ARG A 282 | 19.018 | 29.529 | 31.352 | 1.00 | 72.31 | 6 |
| | ATOM | 150 | NH1 | ARG A 282 | 20.190 | 28.886 | 31.327 | 1.00 | 77.89 | 7 |
| | ATOM | 151 | NH2 | ARG A 282 | 18.802 | 30.593 | 30.595 | 1.00 | 69.25 | 7 |
| 30 | ATOM | 152 | C | ARG A 282 | 19.823 | 29.582 | 37.170 | 1.00 | 34.81 | 6 |
| | ATOM | 153 | O | ARG A 282 | 20.380 | 28.735 | 37.855 | 1.00 | 36.03 | 8 |
| | ATOM | 154 | N | VAL A 283 | 20.135 | 30.882 | 37.190 | 1.00 | 31.71 | 7 |
| | ATOM | 155 | CA | VAL A 283 | 21.171 | 31.434 | 38.057 | 1.00 | 30.16 | 6 |
| | ATOM | 156 | CB | VAL A 283 | 21.198 | 32.965 | 37.981 | 1.00 | 29.00 | 6 |
| 35 | ATOM | 157 | CG1 | VAL A 283 | 22.208 | 33.533 | 38.952 | 1.00 | 28.64 | 6 |
| | ATOM | 158 | CG2 | VAL A 283 | 21.525 | 33.415 | 36.578 | 1.00 | 28.28 | 6 |
| | ATOM | 159 | C | VAL A 283 | 20.942 | 30.992 | 39.498 | 1.00 | 32.50 | 6 |
| | ATOM | 160 | O | VAL A 283 | 21.879 | 30.717 | 40.229 | 1.00 | 33.48 | 8 |
| | ATOM | 161 | N | VAL A 284 | 19.671 | 30.941 | 39.892 | 1.00 | 30.96 | 7 |
| 40 | ATOM | 162 | CA | VAL A 284 | 19.289 | 30.527 | 41.239 | 1.00 | 29.14 | 6 |
| | ATOM | 163 | CB | VAL A 284 | 17.822 | 30.865 | 41.548 | 1.00 | 31.27 | 6 |
| | ATOM | 164 | CG1 | VAL A 284 | 17.472 | 30.461 | 42.945 | 1.00 | 24.21 | 6 |
| | ATOM | 165 | CG2 | VAL A 284 | 17.555 | 32.334 | 41.360 | 1.00 | 30.51 | 6 |
| | ATOM | 166 | C | VAL A 284 | 19.529 | 29.037 | 41.353 | 1.00 | 28.89 | 6 |
| 45 | ATOM | 167 | O | VAL A 284 | 20.073 | 28.568 | 42.345 | 1.00 | 27.29 | 8 |
| | ATOM | 168 | N | ASP A 285 | 19.121 | 28.296 | 40.327 | 1.00 | 28.76 | 7 |
| | ATOM | 169 | CA | ASP A 285 | 19.277 | 26.842 | 40.306 | 1.00 | 35.32 | 6 |
| | ATOM | 170 | CB | ASP A 285 | 18.586 | 26.234 | 39.072 | 1.00 | 33.29 | 6 |
| | ATOM | 171 | CG | ASP A 285 | 17.083 | 26.277 | 39.149 | 1.00 | 38.15 | 6 |
| 50 | ATOM | 172 | OD1 | ASP A 285 | 16.484 | 25.743 | 40.110 | 1.00 | 34.70 | 8 |
| | ATOM | 173 | OD2 | ASP A 285 | 16.431 | 26.828 | 38.231 | 1.00 | 34.43 | 8 |
| | ATOM | 174 | C | ASP A 285 | 20.751 | 26.449 | 40.305 | 1.00 | 36.70 | 6 |
| | ATOM | 175 | O | ASP A 285 | 21.106 | 25.389 | 40.808 | 1.00 | 37.96 | 8 |
| | ATOM | 176 | N | PHE A 286 | 21.604 | 27.300 | 39.737 | 1.00 | 35.96 | 7 |
| 55 | ATOM | 177 | CA | PHE A 286 | 23.029 | 27.022 | 39.704 | 1.00 | 37.10 | 6 |
| | ATOM | 178 | CB | PHE A 286 | 23.754 | 28.009 | 38.793 | 1.00 | 37.97 | 6 |
| | ATOM | 179 | CG | PHE A 286 | 25.252 | 28.027 | 38.987 | 1.00 | 36.50 | 6 |
| | ATOM | 180 | CD1 | PHE A 286 | 25.963 | 26.849 | 38.974 | 1.00 | 36.75 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| 5 | ATOM | 181 | CD2 | PHE | A | 286 | 25.931 | 29.218 | 39.199 | 1.00 | 33.83 | 6 |
| | ATOM | 182 | CE1 | PHE | A | 286 | 27.331 | 26.860 | 39.161 | 1.00 | 39.55 | 6 |
| | ATOM | 183 | CE2 | PHE | A | 286 | 27.307 | 29.233 | 39.387 | 1.00 | 38.08 | 6 |
| | ATOM | 184 | CZ | PHE | A | 286 | 28.008 | 28.052 | 39.371 | 1.00 | 34.44 | 6 |
| | ATOM | 185 | C | PHE | A | 286 | 23.631 | 27.105 | 41.083 | 1.00 | 36.83 | 6 |
| 10 | ATOM | 186 | O | PHE | A | 286 | 24.317 | 26.192 | 41.504 | 1.00 | 35.61 | 8 |
| | ATOM | 187 | N | ALA | A | 287 | 23.393 | 28.228 | 41.752 | 1.00 | 37.33 | 7 |
| | ATOM | 188 | CA | ALA | A | 287 | 23.917 | 28.448 | 43.087 | 1.00 | 36.34 | 6 |
| | ATOM | 189 | CB | ALA | A | 287 | 23.523 | 29.828 | 43.555 | 1.00 | 36.40 | 6 |
| | ATOM | 190 | C | ALA | A | 287 | 23.346 | 27.393 | 44.027 | 1.00 | 38.76 | 6 |
| 15 | ATOM | 191 | O | ALA | A | 287 | 23.994 | 26.973 | 44.981 | 1.00 | 41.98 | 8 |
| | ATOM | 192 | N | LYS | A | 288 | 22.114 | 26.979 | 43.735 | 1.00 | 38.28 | 7 |
| | ATOM | 193 | CA | LYS | A | 288 | 21.429 | 25.971 | 44.538 | 1.00 | 45.26 | 6 |
| | ATOM | 194 | CB | LYS | A | 288 | 19.994 | 25.746 | 44.054 | 1.00 | 48.35 | 6 |
| | ATOM | 195 | CG | LYS | A | 288 | 19.025 | 26.819 | 44.464 | 1.00 | 51.43 | 6 |
| 20 | ATOM | 196 | CD | LYS | A | 288 | 17.628 | 26.246 | 44.682 | 1.00 | 60.23 | 6 |
| | ATOM | 197 | CE | LYS | A | 288 | 17.135 | 25.478 | 43.485 | 1.00 | 62.81 | 6 |
| | ATOM | 198 | NZ | LYS | A | 288 | 17.196 | 26.327 | 42.268 | 1.00 | 64.69 | 7 |
| | ATOM | 199 | C | LYS | A | 288 | 22.120 | 24.632 | 44.536 | 1.00 | 43.31 | 6 |
| | ATOM | 200 | O | LYS | A | 288 | 21.967 | 23.857 | 45.462 | 1.00 | 45.66 | 8 |
| 25 | ATOM | 201 | N | LYS | A | 289 | 22.865 | 24.366 | 43.467 | 1.00 | 41.70 | 7 |
| | ATOM | 202 | CA | LYS | A | 289 | 23.571 | 23.120 | 43.351 | 1.00 | 40.67 | 6 |
| | ATOM | 203 | CB | LYS | A | 289 | 23.655 | 22.708 | 41.877 | 1.00 | 42.25 | 6 |
| | ATOM | 204 | CG | LYS | A | 289 | 22.271 | 22.492 | 41.247 | 1.00 | 39.53 | 6 |
| | ATOM | 205 | CD | LYS | A | 289 | 22.331 | 21.606 | 40.012 | 1.00 | 43.19 | 6 |
| 30 | ATOM | 206 | CE | LYS | A | 289 | 20.941 | 21.362 | 39.447 | 1.00 | 45.74 | 6 |
| | ATOM | 207 | NZ | LYS | A | 289 | 20.273 | 20.165 | 40.006 | 1.00 | 52.49 | 7 |
| | ATOM | 208 | C | LYS | A | 289 | 24.948 | 23.185 | 44.003 | 1.00 | 41.50 | 6 |
| | ATOM | 209 | O | LYS | A | 289 | 25.642 | 22.184 | 44.080 | 1.00 | 39.77 | 8 |
| | ATOM | 210 | N | LEU | A | 290 | 25.312 | 24.370 | 44.490 | 1.00 | 40.68 | 7 |
| 35 | ATOM | 211 | CA | LEU | A | 290 | 26.594 | 24.583 | 45.149 | 1.00 | 39.33 | 6 |
| | ATOM | 212 | CB | LEU | A | 290 | 27.153 | 25.972 | 44.829 | 1.00 | 36.14 | 6 |
| | ATOM | 213 | CG | LEU | A | 290 | 27.358 | 26.290 | 43.365 | 1.00 | 34.81 | 6 |
| | ATOM | 214 | CD1 | LEU | A | 290 | 27.945 | 27.675 | 43.208 | 1.00 | 29.07 | 6 |
| | ATOM | 215 | CD2 | LEU | A | 290 | 28.267 | 25.242 | 42.757 | 1.00 | 33.45 | 6 |
| 40 | ATOM | 216 | C | LEU | A | 290 | 26.434 | 24.405 | 46.652 | 1.00 | 40.08 | 6 |
| | ATOM | 217 | O | LEU | A | 290 | 25.803 | 25.235 | 47.333 | 1.00 | 42.00 | 8 |
| | ATOM | 218 | N | PRO | A | 291 | 27.028 | 23.333 | 47.210 | 1.00 | 40.27 | 7 |
| | ATOM | 219 | CD | PRO | A | 291 | 27.851 | 22.330 | 46.519 | 1.00 | 39.65 | 6 |
| | ATOM | 220 | CA | PRO | A | 291 | 26.905 | 23.096 | 48.659 | 1.00 | 38.28 | 6 |
| 45 | ATOM | 221 | CB | PRO | A | 291 | 27.755 | 21.860 | 48.911 | 1.00 | 35.88 | 6 |
| | ATOM | 222 | CG | PRO | A | 291 | 28.202 | 21.355 | 47.585 | 1.00 | 34.19 | 6 |
| | ATOM | 223 | C | PRO | A | 291 | 27.327 | 24.298 | 49.522 | 1.00 | 40.05 | 6 |
| | ATOM | 224 | O | PRO | A | 291 | 26.571 | 24.739 | 50.391 | 1.00 | 41.33 | 8 |
| | ATOM | 225 | N | MET | A | 292 | 28.522 | 24.843 | 49.299 | 1.00 | 40.59 | 7 |
| 50 | ATOM | 226 | CA | MET | A | 292 | 29.021 | 25.957 | 50.097 | 1.00 | 42.86 | 6 |
| | ATOM | 227 | CB | MET | A | 292 | 30.313 | 26.475 | 49.477 | 1.00 | 43.28 | 6 |
| | ATOM | 228 | CG | MET | A | 292 | 31.269 | 25.378 | 49.050 | 1.00 | 50.35 | 6 |
| | ATOM | 229 | SD | MET | A | 292 | 32.895 | 26.096 | 48.757 | 1.00 | 51.17 | 16 |
| | ATOM | 230 | CE | MET | A | 292 | 33.812 | 24.647 | 48.074 | 1.00 | 54.63 | 6 |
| 55 | ATOM | 231 | C | MET | A | 292 | 27.984 | 27.066 | 50.149 | 1.00 | 41.05 | 6 |
| | ATOM | 232 | O | MET | A | 292 | 27.986 | 27.886 | 51.057 | 1.00 | 39.66 | 8 |
| | ATOM | 233 | N | PHE | A | 293 | 27.080 | 27.078 | 49.172 | 1.00 | 39.30 | 7 |
| | ATOM | 234 | CA | PHE | A | 293 | 26.030 | 28.091 | 49.114 | 1.00 | 40.92 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| 5 | ATOM | 235 | CB | PHE | A | 293 | 25.398 | 28.111 | 47.715 | 1.00 | 40.98 | 6 |
| | ATOM | 236 | CG | PHE | A | 293 | 24.348 | 29.168 | 47.524 | 1.00 | 42.78 | 6 |
| | ATOM | 237 | CD1 | PHE | A | 293 | 24.654 | 30.493 | 47.747 | 1.00 | 44.40 | 6 |
| | ATOM | 238 | CD2 | PHE | A | 293 | 23.071 | 28.833 | 47.116 | 1.00 | 43.66 | 6 |
| | ATOM | 239 | CE1 | PHE | A | 293 | 23.701 | 31.478 | 47.564 | 1.00 | 39.83 | 6 |
| 10 | ATOM | 240 | CE2 | PHE | A | 293 | 22.112 | 29.819 | 46.930 | 1.00 | 46.21 | 6 |
| | ATOM | 241 | CZ | PHE | A | 293 | 22.430 | 31.146 | 47.155 | 1.00 | 45.18 | 6 |
| | ATOM | 242 | C | PHE | A | 293 | 24.979 | 27.772 | 50.164 | 1.00 | 45.54 | 6 |
| | ATOM | 243 | O | PHE | A | 293 | 24.686 | 28.576 | 51.034 | 1.00 | 42.01 | 8 |
| | ATOM | 244 | N | CYS | A | 294 | 24.426 | 26.572 | 50.062 | 1.00 | 47.05 | 7 |
| 15 | ATOM | 245 | CA | CYS | A | 294 | 23.386 | 26.125 | 50.962 | 1.00 | 50.15 | 6 |
| | ATOM | 246 | CB | CYS | A | 294 | 22.944 | 24.733 | 50.524 | 1.00 | 45.90 | 6 |
| | ATOM | 247 | SG | CYS | A | 294 | 22.303 | 24.663 | 48.829 | 1.00 | 51.50 | 16 |
| | ATOM | 248 | C | CYS | A | 294 | 23.825 | 26.125 | 52.423 | 1.00 | 51.38 | 6 |
| | ATOM | 249 | O | CYS | A | 294 | 23.008 | 25.954 | 53.322 | 1.00 | 53.83 | 8 |
| 20 | ATOM | 250 | N | GLU | A | 295 | 25.119 | 26.327 | 52.645 | 1.00 | 49.72 | 7 |
| | ATOM | 251 | CA | GLU | A | 295 | 25.666 | 26.384 | 53.996 | 1.00 | 52.53 | 6 |
| | ATOM | 252 | CB | GLU | A | 295 | 27.103 | 25.830 | 54.015 | 1.00 | 57.40 | 6 |
| | ATOM | 253 | CG | GLU | A | 295 | 27.182 | 24.309 | 54.061 | 1.00 | 69.63 | 6 |
| | ATOM | 254 | CD | GLU | A | 295 | 26.660 | 23.747 | 55.342 | 1.00 | 78.49 | 6 |
| 25 | ATOM | 255 | OE1 | GLU | A | 295 | 27.291 | 23.946 | 56.412 | 1.00 | 82.82 | 8 |
| | ATOM | 256 | OE2 | GLU | A | 295 | 25.590 | 23.086 | 55.335 | 1.00 | 85.30 | 8 |
| | ATOM | 257 | C | GLU | A | 295 | 25.653 | 27.831 | 54.488 | 1.00 | 48.54 | 6 |
| | ATOM | 258 | O | GLU | A | 295 | 26.365 | 28.184 | 55.426 | 1.00 | 49.82 | 8 |
| | ATOM | 259 | N | LEU | A | 296 | 24.804 | 28.631 | 53.846 | 1.00 | 43.79 | 7 |
| 30 | ATOM | 260 | CA | LEU | A | 296 | 24.670 | 30.034 | 54.159 | 1.00 | 45.42 | 6 |
| | ATOM | 261 | CB | LEU | A | 296 | 25.062 | 30.864 | 52.923 | 1.00 | 41.04 | 6 |
| | ATOM | 262 | CG | LEU | A | 296 | 26.438 | 30.658 | 52.315 | 1.00 | 42.74 | 6 |
| | ATOM | 263 | CD1 | LEU | A | 296 | 26.447 | 31.030 | 50.861 | 1.00 | 40.99 | 6 |
| | ATOM | 264 | CD2 | LEU | A | 296 | 27.437 | 31.454 | 53.086 | 1.00 | 39.44 | 6 |
| 35 | ATOM | 265 | C | LEU | A | 296 | 23.239 | 30.366 | 54.548 | 1.00 | 45.56 | 6 |
| | ATOM | 266 | O | LEU | A | 296 | 22.301 | 29.660 | 54.148 | 1.00 | 43.07 | 8 |
| | ATOM | 267 | N | PRO | A | 297 | 23.050 | 31.405 | 55.365 | 1.00 | 46.99 | 7 |
| | ATOM | 268 | CD | PRO | A | 297 | 24.121 | 32.241 | 55.930 | 1.00 | 47.12 | 6 |
| | ATOM | 269 | CA | PRO | A | 297 | 21.700 | 31.811 | 55.787 | 1.00 | 49.61 | 6 |
| 40 | ATOM | 270 | CB | PRO | A | 297 | 21.937 | 32.990 | 56.738 | 1.00 | 49.91 | 6 |
| | ATOM | 271 | CG | PRO | A | 297 | 23.401 | 33.155 | 56.872 | 1.00 | 51.28 | 6 |
| | ATOM | 272 | C | PRO | A | 297 | 20.864 | 32.212 | 54.558 | 1.00 | 49.59 | 6 |
| | ATOM | 273 | O | PRO | A | 297 | 21.402 | 32.684 | 53.556 | 1.00 | 51.66 | 8 |
| | ATOM | 274 | N | CYS | A | 298 | 19.545 | 32.035 | 54.655 | 1.00 | 51.02 | 7 |
| 45 | ATOM | 275 | CA | CYS | A | 298 | 18.618 | 32.369 | 53.567 | 1.00 | 52.86 | 6 |
| | ATOM | 276 | CB | CYS | A | 298 | 17.201 | 31.877 | 53.915 | 1.00 | 54.57 | 6 |
| | ATOM | 277 | SG | CYS | A | 298 | 16.040 | 33.162 | 54.440 | 1.00 | 67.87 | 16 |
| | ATOM | 278 | C | CYS | A | 298 | 18.583 | 33.863 | 53.291 | 1.00 | 48.51 | 6 |
| | ATOM | 279 | O | CYS | A | 298 | 18.039 | 34.288 | 52.282 | 1.00 | 49.58 | 8 |
| 50 | ATOM | 280 | N | GLU | A | 299 | 19.144 | 34.654 | 54.202 | 1.00 | 44.17 | 7 |
| | ATOM | 281 | CA | GLU | A | 299 | 19.179 | 36.096 | 54.016 | 1.00 | 47.57 | 6 |
| | ATOM | 282 | CB | GLU | A | 299 | 19.265 | 36.833 | 55.360 | 1.00 | 49.92 | 6 |
| | ATOM | 283 | CG | GLU | A | 299 | 17.931 | 36.996 | 56.125 | 1.00 | 59.30 | 6 |
| | ATOM | 284 | CD | GLU | A | 299 | 17.613 | 35.904 | 57.095 | 1.00 | 63.80 | 6 |
| 55 | ATOM | 285 | OE1 | GLU | A | 299 | 16.512 | 35.952 | 57.706 | 1.00 | 69.03 | 8 |
| | ATOM | 286 | OE2 | GLU | A | 299 | 18.436 | 34.976 | 57.292 | 1.00 | 67.10 | 8 |
| | ATOM | 287 | C | GLU | A | 299 | 20.359 | 36.492 | 53.152 | 1.00 | 46.57 | 6 |
| | ATOM | 288 | O | GLU | A | 299 | 20.265 | 37.441 | 52.379 | 1.00 | 44.65 | 8 |

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|----|------|-----|-----|-------|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 289 | N | ASP A | 300 | 21.467 | 35.763 | 52.294 | 1.00 | 43.32 | 7 |
| | ATOM | 290 | CA | ASP A | 300 | 22.661 | 36.042 | 52.509 | 1.00 | 43.32 | 6 |
| | ATOM | 291 | CB | ASP A | 300 | 23.919 | 35.513 | 53.213 | 1.00 | 37.38 | 6 |
| | ATOM | 292 | CG | ASP A | 300 | 24.223 | 36.239 | 54.473 | 1.00 | 36.23 | 6 |
| | ATOM | 293 | OD1 | ASP A | 300 | 24.153 | 37.488 | 54.493 | 1.00 | 35.87 | 8 |
| 10 | ATOM | 294 | OD2 | ASP A | 300 | 24.572 | 35.575 | 55.483 | 1.00 | 40.14 | 8 |
| | ATOM | 295 | C | ASP A | 300 | 22.514 | 35.390 | 51.138 | 1.00 | 42.81 | 6 |
| | ATOM | 296 | O | ASP A | 300 | 22.775 | 36.021 | 50.113 | 1.00 | 46.02 | 8 |
| | ATOM | 297 | N | GLN A | 301 | 22.095 | 34.124 | 51.137 | 1.00 | 38.60 | 7 |
| | ATOM | 298 | CA | GLN A | 301 | 21.896 | 33.390 | 49.902 | 1.00 | 40.00 | 6 |
| 15 | ATOM | 299 | CB | GLN A | 301 | 20.991 | 32.179 | 50.137 | 1.00 | 38.59 | 6 |
| | ATOM | 300 | CG | GLN A | 301 | 21.644 | 31.003 | 50.808 | 1.00 | 40.26 | 6 |
| | ATOM | 301 | CD | GLN A | 301 | 20.690 | 29.824 | 50.988 | 1.00 | 44.15 | 6 |
| | ATOM | 302 | OE1 | GLN A | 301 | 19.658 | 29.957 | 51.675 | 1.00 | 45.73 | 8 |
| | ATOM | 303 | NE2 | GLN A | 301 | 21.027 | 28.685 | 50.394 | 1.00 | 46.13 | 7 |
| 20 | ATOM | 304 | C | GLN A | 301 | 21.242 | 34.305 | 48.877 | 1.00 | 41.64 | 6 |
| | ATOM | 305 | O | GLN A | 301 | 21.482 | 34.185 | 47.686 | 1.00 | 45.02 | 8 |
| | ATOM | 306 | N | ILE A | 302 | 20.413 | 35.228 | 49.372 | 1.00 | 41.01 | 7 |
| | ATOM | 307 | CA | ILE A | 302 | 19.726 | 36.179 | 48.511 | 1.00 | 40.23 | 6 |
| | ATOM | 308 | CB | ILE A | 302 | 18.502 | 36.774 | 49.217 | 1.00 | 39.52 | 6 |
| 25 | ATOM | 309 | CG2 | ILE A | 302 | 17.818 | 37.788 | 48.342 | 1.00 | 31.98 | 6 |
| | ATOM | 310 | CG1 | ILE A | 302 | 17.502 | 35.673 | 49.581 | 1.00 | 40.77 | 6 |
| | ATOM | 311 | CD1 | ILE A | 302 | 17.003 | 34.897 | 48.385 | 1.00 | 45.43 | 6 |
| | ATOM | 312 | C | ILE A | 302 | 20.698 | 37.268 | 48.096 | 1.00 | 38.58 | 6 |
| | ATOM | 313 | O | ILE A | 302 | 20.960 | 37.453 | 46.906 | 1.00 | 40.81 | 8 |
| 30 | ATOM | 314 | N | ILE A | 303 | 21.228 | 37.972 | 49.097 | 1.00 | 37.50 | 7 |
| | ATOM | 315 | CA | ILE A | 303 | 22.179 | 39.060 | 48.874 | 1.00 | 39.33 | 6 |
| | ATOM | 316 | CB | ILE A | 303 | 23.023 | 39.338 | 50.109 | 1.00 | 39.06 | 6 |
| | ATOM | 317 | CG2 | ILE A | 303 | 23.946 | 40.522 | 49.861 | 1.00 | 36.19 | 6 |
| | ATOM | 318 | CG1 | ILE A | 303 | 22.141 | 39.653 | 51.313 | 1.00 | 40.15 | 6 |
| 35 | ATOM | 319 | CD1 | ILE A | 303 | 22.916 | 39.806 | 52.589 | 1.00 | 36.93 | 6 |
| | ATOM | 320 | C | ILE A | 303 | 23.093 | 38.705 | 47.722 | 1.00 | 36.49 | 6 |
| | ATOM | 321 | O | ILE A | 303 | 23.354 | 39.509 | 46.835 | 1.00 | 36.58 | 8 |
| | ATOM | 322 | N | LEU A | 304 | 23.580 | 37.477 | 47.762 | 1.00 | 32.91 | 7 |
| | ATOM | 323 | CA | LEU A | 304 | 24.465 | 36.964 | 46.734 | 1.00 | 27.55 | 6 |
| 40 | ATOM | 324 | CB | LEU A | 304 | 24.935 | 35.554 | 47.123 | 1.00 | 22.35 | 6 |
| | ATOM | 325 | CG | LEU A | 304 | 26.150 | 35.480 | 48.029 | 1.00 | 26.88 | 6 |
| | ATOM | 326 | CD1 | LEU A | 304 | 26.267 | 36.731 | 48.876 | 1.00 | 24.82 | 6 |
| | ATOM | 327 | CD2 | LEU A | 304 | 26.084 | 34.226 | 48.861 | 1.00 | 23.69 | 6 |
| | ATOM | 328 | C | LEU A | 304 | 23.764 | 36.968 | 45.389 | 1.00 | 28.05 | 6 |
| 45 | ATOM | 329 | O | LEU A | 304 | 24.212 | 37.623 | 44.443 | 1.00 | 24.68 | 8 |
| | ATOM | 330 | N | LEU A | 305 | 22.657 | 36.236 | 45.318 | 1.00 | 26.34 | 7 |
| | ATOM | 331 | CA | LEU A | 305 | 21.892 | 36.147 | 44.089 | 1.00 | 30.91 | 6 |
| | ATOM | 332 | CB | LEU A | 305 | 20.565 | 35.434 | 44.359 | 1.00 | 32.50 | 6 |
| | ATOM | 333 | CG | LEU A | 305 | 20.637 | 33.950 | 44.635 | 1.00 | 33.36 | 6 |
| 50 | ATOM | 334 | CD1 | LEU A | 305 | 19.247 | 33.370 | 44.779 | 1.00 | 33.87 | 6 |
| | ATOM | 335 | CD2 | LEU A | 305 | 21.340 | 33.280 | 43.466 | 1.00 | 31.72 | 6 |
| | ATOM | 336 | C | LEU A | 305 | 21.665 | 37.524 | 43.477 | 1.00 | 29.76 | 6 |
| | ATOM | 337 | O | LEU A | 305 | 21.954 | 37.747 | 42.301 | 1.00 | 29.33 | 8 |
| | ATOM | 338 | N | LYS A | 306 | 21.157 | 38.439 | 44.298 | 1.00 | 29.72 | 7 |
| 55 | ATOM | 339 | CA | LYS A | 306 | 20.868 | 39.800 | 43.864 | 1.00 | 34.28 | 6 |
| | ATOM | 340 | CB | LYS A | 306 | 20.293 | 40.615 | 45.026 | 1.00 | 35.98 | 6 |
| | ATOM | 341 | CG | LYS A | 306 | 18.919 | 40.163 | 45.511 | 1.00 | 43.35 | 6 |
| | ATOM | 342 | CD | LYS A | 306 | 18.397 | 41.127 | 46.559 | 1.00 | 51.50 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| 5 | ATOM | 343 | CE | LYS | A | 306 | 18.271 | 42.515 | 45.971 | 1.00 | 53.26 | 6 |
| | ATOM | 344 | NZ | LYS | A | 306 | 18.325 | 43.548 | 47.038 | 1.00 | 59.61 | 7 |
| | ATOM | 345 | C | LYS | A | 306 | 22.075 | 40.527 | 43.302 | 1.00 | 35.25 | 6 |
| | ATOM | 346 | O | LYS | A | 306 | 21.972 | 41.286 | 42.334 | 1.00 | 33.95 | 8 |
| | ATOM | 347 | N | GLY | A | 307 | 23.228 | 40.306 | 43.928 | 1.00 | 35.79 | 7 |
| 10 | ATOM | 348 | CA | GLY | A | 307 | 24.445 | 40.962 | 43.482 | 1.00 | 34.59 | 6 |
| | ATOM | 349 | C | GLY | A | 307 | 25.109 | 40.353 | 42.259 | 1.00 | 33.80 | 6 |
| | ATOM | 350 | O | GLY | A | 307 | 25.489 | 41.087 | 41.344 | 1.00 | 31.59 | 8 |
| | ATOM | 351 | N | CYS | A | 308 | 25.248 | 39.024 | 42.256 | 1.00 | 31.15 | 7 |
| | ATOM | 352 | CA | CYS | A | 308 | 25.899 | 38.326 | 41.174 | 1.00 | 29.04 | 6 |
| 15 | ATOM | 353 | CB | CYS | A | 308 | 26.604 | 37.089 | 41.704 | 1.00 | 27.59 | 6 |
| | ATOM | 354 | SG | CYS | A | 308 | 25.472 | 35.770 | 42.071 | 1.00 | 30.50 | 16 |
| | ATOM | 355 | C | CYS | A | 308 | 24.974 | 37.870 | 40.062 | 1.00 | 30.59 | 6 |
| | ATOM | 356 | O | CYS | A | 308 | 25.458 | 37.319 | 39.077 | 1.00 | 33.77 | 8 |
| | ATOM | 357 | N | CYS | A | 309 | 23.664 | 38.084 | 40.195 | 1.00 | 28.46 | 7 |
| 20 | ATOM | 358 | CA | CYS | A | 309 | 22.739 | 37.623 | 39.168 | 1.00 | 30.10 | 6 |
| | ATOM | 359 | CB | CYS | A | 309 | 21.311 | 38.004 | 39.490 | 1.00 | 33.43 | 6 |
| | ATOM | 360 | SG | CYS | A | 309 | 20.198 | 37.299 | 38.307 | 1.00 | 35.20 | 16 |
| | ATOM | 361 | C | CYS | A | 309 | 23.065 | 38.123 | 37.788 | 1.00 | 27.72 | 6 |
| | ATOM | 362 | O | CYS | A | 309 | 23.212 | 37.334 | 36.865 | 1.00 | 27.69 | 8 |
| 25 | ATOM | 363 | N | MET | A | 310 | 23.157 | 39.439 | 37.639 | 1.00 | 26.15 | 7 |
| | ATOM | 364 | CA | MET | A | 310 | 23.476 | 40.016 | 36.342 | 1.00 | 26.06 | 6 |
| | ATOM | 365 | CB | MET | A | 310 | 23.482 | 41.547 | 36.419 | 1.00 | 25.32 | 6 |
| | ATOM | 366 | CG | MET | A | 310 | 23.913 | 42.230 | 35.109 | 1.00 | 24.08 | 6 |
| | ATOM | 367 | SD | MET | A | 310 | 22.765 | 41.751 | 33.762 | 1.00 | 27.71 | 16 |
| 30 | ATOM | 368 | CE | MET | A | 310 | 23.650 | 42.321 | 32.270 | 1.00 | 28.50 | 6 |
| | ATOM | 369 | C | MET | A | 310 | 24.842 | 39.527 | 35.908 | 1.00 | 25.94 | 6 |
| | ATOM | 370 | O | MET | A | 310 | 25.020 | 39.076 | 34.788 | 1.00 | 28.09 | 8 |
| | ATOM | 371 | N | GLU | A | 311 | 25.800 | 39.638 | 36.826 | 1.00 | 25.39 | 7 |
| | ATOM | 372 | CA | GLU | A | 311 | 27.176 | 39.234 | 36.589 | 1.00 | 27.03 | 6 |
| 35 | ATOM | 373 | CB | GLU | A | 311 | 27.973 | 39.303 | 37.900 | 1.00 | 24.39 | 6 |
| | ATOM | 374 | CG | GLU | A | 311 | 27.842 | 40.628 | 38.668 | 1.00 | 26.00 | 6 |
| | ATOM | 375 | CD | GLU | A | 311 | 28.726 | 40.720 | 39.870 | 1.00 | 23.95 | 6 |
| | ATOM | 376 | OE1 | GLU | A | 311 | 28.891 | 39.706 | 40.588 | 1.00 | 19.72 | 8 |
| | ATOM | 377 | OE2 | GLU | A | 311 | 29.270 | 41.818 | 40.159 | 1.00 | 26.51 | 8 |
| 40 | ATOM | 378 | C | GLU | A | 311 | 27.266 | 37.827 | 35.997 | 1.00 | 27.51 | 6 |
| | ATOM | 379 | O | GLU | A | 311 | 27.956 | 37.620 | 35.014 | 1.00 | 29.67 | 8 |
| | ATOM | 380 | N | ILE | A | 312 | 26.569 | 36.866 | 36.602 | 1.00 | 26.82 | 7 |
| | ATOM | 381 | CA | ILE | A | 312 | 26.593 | 35.497 | 36.112 | 1.00 | 25.71 | 6 |
| | ATOM | 382 | CB | ILE | A | 312 | 25.991 | 34.518 | 37.123 | 1.00 | 23.35 | 6 |
| 45 | ATOM | 383 | CG2 | ILE | A | 312 | 25.917 | 33.123 | 36.533 | 1.00 | 20.27 | 6 |
| | ATOM | 384 | CG1 | ILE | A | 312 | 26.837 | 34.471 | 38.398 | 1.00 | 20.88 | 6 |
| | ATOM | 385 | CD1 | ILE | A | 312 | 26.462 | 33.342 | 39.341 | 1.00 | 18.15 | 6 |
| | ATOM | 386 | C | ILE | A | 312 | 25.871 | 35.371 | 34.791 | 1.00 | 27.91 | 6 |
| | ATOM | 387 | O | ILE | A | 312 | 26.274 | 34.593 | 33.934 | 1.00 | 28.96 | 8 |
| 50 | ATOM | 388 | N | MET | A | 313 | 24.788 | 36.130 | 34.633 | 1.00 | 27.66 | 7 |
| | ATOM | 389 | CA | MET | A | 313 | 24.013 | 36.081 | 33.395 | 1.00 | 30.18 | 6 |
| | ATOM | 390 | CB | MET | A | 313 | 22.716 | 36.888 | 33.508 | 1.00 | 36.89 | 6 |
| | ATOM | 391 | CG | MET | A | 313 | 21.608 | 36.198 | 34.305 | 1.00 | 37.95 | 6 |
| | ATOM | 392 | SD | MET | A | 313 | 19.892 | 36.817 | 34.055 | 1.00 | 42.38 | 16 |
| 55 | ATOM | 393 | CE | MET | A | 313 | 20.034 | 38.503 | 34.740 | 1.00 | 40.68 | 6 |
| | ATOM | 394 | C | MET | A | 313 | 24.834 | 36.579 | 32.222 | 1.00 | 27.43 | 6 |
| | ATOM | 395 | O | MET | A | 313 | 25.116 | 35.814 | 31.308 | 1.00 | 28.61 | 8 |
| | ATOM | 396 | N | SER | A | 314 | 25.209 | 37.859 | 32.253 | 1.00 | 24.88 | 7 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 397 | CA | SER | A | 314 | 26.005 | 38.472 | 31.197 | 1.00 | 27.98 | 6 |
| | ATOM | 398 | CB | SER | A | 314 | 26.354 | 39.914 | 31.581 | 1.00 | 29.64 | 6 |
| | ATOM | 399 | OG | SER | A | 314 | 26.956 | 39.972 | 32.858 | 1.00 | 43.44 | 8 |
| | ATOM | 400 | C | SER | A | 314 | 27.275 | 37.679 | 30.851 | 1.00 | 22.30 | 6 |
| | ATOM | 401 | O | SER | A | 314 | 27.675 | 37.629 | 29.690 | 1.00 | 24.18 | 8 |
| 10 | ATOM | 402 | N | LEU | A | 315 | 27.905 | 37.048 | 31.845 | 1.00 | 23.99 | 7 |
| | ATOM | 403 | CA | LEU | A | 315 | 29.099 | 36.261 | 31.563 | 1.00 | 25.07 | 6 |
| | ATOM | 404 | CB | LEU | A | 315 | 29.685 | 35.593 | 32.816 | 1.00 | 19.11 | 6 |
| | ATOM | 405 | CG | LEU | A | 315 | 30.675 | 34.479 | 32.505 | 1.00 | 20.39 | 6 |
| | ATOM | 406 | CD1 | LEU | A | 315 | 31.866 | 35.040 | 31.756 | 1.00 | 18.92 | 6 |
| 15 | ATOM | 407 | CD2 | LEU | A | 315 | 31.125 | 33.789 | 33.765 | 1.00 | 12.93 | 6 |
| | ATOM | 408 | C | LEU | A | 315 | 28.700 | 35.180 | 30.597 | 1.00 | 24.53 | 6 |
| | ATOM | 409 | O | LEU | A | 315 | 29.304 | 35.036 | 29.556 | 1.00 | 26.32 | 8 |
| | ATOM | 410 | N | ARG | A | 316 | 27.678 | 34.426 | 30.982 | 1.00 | 28.18 | 7 |
| | ATOM | 411 | CA | ARG | A | 316 | 27.151 | 33.312 | 30.216 | 1.00 | 27.54 | 6 |
| 20 | ATOM | 412 | CB | ARG | A | 316 | 25.915 | 32.752 | 30.928 | 1.00 | 27.39 | 6 |
| | ATOM | 413 | CG | ARG | A | 316 | 26.188 | 32.190 | 32.336 | 1.00 | 22.00 | 6 |
| | ATOM | 414 | CD | ARG | A | 316 | 24.934 | 31.526 | 32.901 | 1.00 | 18.78 | 6 |
| | ATOM | 415 | NE | ARG | A | 316 | 25.245 | 30.376 | 33.721 | 1.00 | 26.57 | 7 |
| | ATOM | 416 | CZ | ARG | A | 316 | 24.341 | 29.468 | 34.054 | 1.00 | 30.81 | 6 |
| 25 | ATOM | 417 | NH1 | ARG | A | 316 | 23.084 | 29.614 | 33.639 | 1.00 | 33.71 | 7 |
| | ATOM | 418 | NH2 | ARG | A | 316 | 24.701 | 28.416 | 34.776 | 1.00 | 33.13 | 7 |
| | ATOM | 419 | C | ARG | A | 316 | 26.774 | 33.660 | 28.794 | 1.00 | 28.09 | 6 |
| | ATOM | 420 | O | ARG | A | 316 | 26.737 | 32.792 | 27.931 | 1.00 | 32.41 | 8 |
| | ATOM | 421 | N | ALA | A | 317 | 26.484 | 34.936 | 28.571 | 1.00 | 28.36 | 7 |
| 30 | ATOM | 422 | CA | ALA | A | 317 | 26.094 | 35.411 | 27.264 | 1.00 | 26.64 | 6 |
| | ATOM | 423 | CB | ALA | A | 317 | 25.232 | 36.666 | 27.418 | 1.00 | 22.93 | 6 |
| | ATOM | 424 | C | ALA | A | 317 | 27.323 | 35.714 | 26.417 | 1.00 | 28.35 | 6 |
| | ATOM | 425 | O | ALA | A | 317 | 27.398 | 35.342 | 25.252 | 1.00 | 32.10 | 8 |
| | ATOM | 426 | N | ALA | A | 318 | 28.286 | 36.396 | 27.026 | 1.00 | 29.12 | 7 |
| 35 | ATOM | 427 | CA | ALA | A | 318 | 29.515 | 36.760 | 26.350 | 1.00 | 27.50 | 6 |
| | ATOM | 428 | CB | ALA | A | 318 | 30.434 | 37.452 | 27.333 | 1.00 | 28.39 | 6 |
| | ATOM | 429 | C | ALA | A | 318 | 30.181 | 35.502 | 25.825 | 1.00 | 28.10 | 6 |
| | ATOM | 430 | O | ALA | A | 318 | 30.600 | 35.447 | 24.678 | 1.00 | 28.18 | 8 |
| | ATOM | 431 | N | VAL | A | 319 | 30.255 | 34.491 | 26.700 | 1.00 | 29.16 | 7 |
| 40 | ATOM | 432 | CA | VAL | A | 319 | 30.880 | 33.198 | 26.393 | 1.00 | 35.24 | 6 |
| | ATOM | 433 | CB | VAL | A | 319 | 30.703 | 32.210 | 27.547 | 1.00 | 27.34 | 6 |
| | ATOM | 434 | CG1 | VAL | A | 319 | 30.895 | 32.891 | 28.858 | 1.00 | 29.96 | 6 |
| | ATOM | 435 | CG2 | VAL | A | 319 | 29.353 | 31.552 | 27.482 | 1.00 | 31.70 | 6 |
| | ATOM | 436 | C | VAL | A | 319 | 30.215 | 32.608 | 25.165 | 1.00 | 40.01 | 6 |
| 45 | ATOM | 437 | O | VAL | A | 319 | 30.640 | 31.575 | 24.680 | 1.00 | 42.70 | 8 |
| | ATOM | 438 | N | ARG | A | 320 | 29.176 | 33.284 | 24.683 | 1.00 | 38.64 | 7 |
| | ATOM | 439 | CA | ARG | A | 320 | 28.415 | 32.822 | 23.545 | 1.00 | 38.61 | 6 |
| | ATOM | 440 | CB | ARG | A | 320 | 27.031 | 32.458 | 24.043 | 1.00 | 37.26 | 6 |
| | ATOM | 441 | CG | ARG | A | 320 | 26.863 | 30.991 | 24.192 | 1.00 | 43.12 | 6 |
| 50 | ATOM | 442 | CD | ARG | A | 320 | 25.637 | 30.642 | 25.014 | 1.00 | 50.79 | 6 |
| | ATOM | 443 | NE | ARG | A | 320 | 25.258 | 29.256 | 24.770 | 1.00 | 54.71 | 7 |
| | ATOM | 444 | CZ | ARG | A | 320 | 24.331 | 28.625 | 25.501 | 1.00 | 57.89 | 6 |
| | ATOM | 445 | NH1 | ARG | A | 320 | 23.667 | 29.291 | 26.440 | 1.00 | 49.08 | 7 |
| | ATOM | 446 | NH2 | ARG | A | 320 | 23.964 | 27.385 | 25.242 | 1.00 | 59.59 | 7 |
| 55 | ATOM | 447 | C | ARG | A | 320 | 28.292 | 33.825 | 22.405 | 1.00 | 42.14 | 6 |
| | ATOM | 448 | O | ARG | A | 320 | 27.251 | 33.909 | 21.748 | 1.00 | 46.30 | 8 |
| | ATOM | 449 | N | TYR | A | 321 | 29.352 | 34.583 | 22.173 | 1.00 | 42.04 | 7 |
| | ATOM | 450 | CA | TYR | A | 321 | 29.366 | 35.555 | 21.098 | 1.00 | 42.70 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 451 | CB | TYR | A | 321 | 30.083 | 36.810 | 21.575 | 1.00 | 38.01 | 6 |
| | ATOM | 452 | CG | TYR | A | 321 | 30.601 | 37.650 | 20.448 | 1.00 | 37.94 | 6 |
| | ATOM | 453 | CD1 | TYR | A | 321 | 29.733 | 38.296 | 19.574 | 1.00 | 33.85 | 6 |
| | ATOM | 454 | CE1 | TYR | A | 321 | 30.235 | 39.037 | 18.494 | 1.00 | 34.49 | 6 |
| | ATOM | 455 | CD2 | TYR | A | 321 | 31.966 | 37.743 | 20.224 | 1.00 | 28.03 | 6 |
| 10 | ATOM | 456 | CE2 | TYR | A | 321 | 32.473 | 38.475 | 19.153 | 1.00 | 32.69 | 6 |
| | ATOM | 457 | CZ | TYR | A | 321 | 31.612 | 39.125 | 18.276 | 1.00 | 35.18 | 6 |
| | ATOM | 458 | OH | TYR | A | 321 | 32.107 | 39.866 | 17.223 | 1.00 | 39.48 | 8 |
| | ATOM | 459 | C | TYR | A | 321 | 30.085 | 35.005 | 19.877 | 1.00 | 45.51 | 6 |
| | ATOM | 460 | O | TYR | A | 321 | 31.261 | 34.697 | 19.951 | 1.00 | 48.02 | 8 |
| 15 | ATOM | 461 | N | ASP | A | 322 | 29.354 | 34.879 | 18.773 | 1.00 | 44.56 | 7 |
| | ATOM | 462 | CA | ASP | A | 322 | 29.912 | 34.400 | 17.502 | 1.00 | 45.86 | 6 |
| | ATOM | 463 | CB | ASP | A | 322 | 28.804 | 33.670 | 16.736 | 1.00 | 46.64 | 6 |
| | ATOM | 464 | CG | ASP | A | 322 | 29.050 | 33.608 | 15.255 | 1.00 | 40.00 | 6 |
| | ATOM | 465 | OD1 | ASP | A | 322 | 30.010 | 34.256 | 14.768 | 1.00 | 40.00 | 8 |
| 20 | ATOM | 466 | OD2 | ASP | A | 322 | 28.262 | 32.929 | 14.536 | 1.00 | 40.00 | 8 |
| | ATOM | 467 | C | ASP | A | 322 | 30.460 | 35.629 | 16.755 | 1.00 | 45.82 | 6 |
| | ATOM | 468 | O | ASP | A | 322 | 29.678 | 36.464 | 16.271 | 1.00 | 45.38 | 8 |
| | ATOM | 469 | N | PRO | A | 323 | 31.800 | 35.735 | 16.584 | 1.00 | 46.53 | 7 |
| | ATOM | 470 | CD | PRO | A | 323 | 32.774 | 34.719 | 16.991 | 1.00 | 47.16 | 6 |
| 25 | ATOM | 471 | CA | PRO | A | 323 | 32.424 | 36.889 | 15.890 | 1.00 | 46.63 | 6 |
| | ATOM | 472 | CB | PRO | A | 323 | 33.921 | 36.603 | 15.936 | 1.00 | 43.95 | 6 |
| | ATOM | 473 | CG | PRO | A | 323 | 34.099 | 35.303 | 16.582 | 1.00 | 43.93 | 6 |
| | ATOM | 474 | C | PRO | A | 323 | 31.953 | 37.087 | 14.453 | 1.00 | 48.34 | 6 |
| | ATOM | 475 | O | PRO | A | 323 | 31.797 | 38.210 | 13.960 | 1.00 | 50.84 | 8 |
| 30 | ATOM | 476 | N | GLU | A | 324 | 31.778 | 35.970 | 13.752 | 1.00 | 52.39 | 7 |
| | ATOM | 477 | CA | GLU | A | 324 | 31.339 | 35.968 | 12.370 | 1.00 | 55.85 | 6 |
| | ATOM | 478 | CB | GLU | A | 324 | 31.035 | 34.528 | 11.965 | 1.00 | 55.54 | 6 |
| | ATOM | 479 | CG | GLU | A | 324 | 32.224 | 33.584 | 12.104 | 1.00 | 40.00 | 6 |
| | ATOM | 480 | CD | GLU | A | 324 | 33.432 | 34.023 | 11.310 | 1.00 | 40.00 | 6 |
| 35 | ATOM | 481 | OE1 | GLU | A | 324 | 33.350 | 35.040 | 10.555 | 1.00 | 40.00 | 8 |
| | ATOM | 482 | OE2 | GLU | A | 324 | 34.506 | 33.356 | 11.415 | 1.00 | 40.00 | 8 |
| | ATOM | 483 | C | GLU | A | 324 | 30.077 | 36.798 | 12.277 | 1.00 | 54.94 | 6 |
| | ATOM | 484 | O | GLU | A | 324 | 30.070 | 37.892 | 11.730 | 1.00 | 59.81 | 8 |
| | ATOM | 485 | N | SER | A | 325 | 29.009 | 36.212 | 12.810 | 1.00 | 52.95 | 7 |
| 40 | ATOM | 486 | CA | SER | A | 325 | 27.695 | 36.812 | 12.839 | 1.00 | 50.10 | 6 |
| | ATOM | 487 | CB | SER | A | 325 | 26.701 | 35.797 | 13.402 | 1.00 | 48.23 | 6 |
| | ATOM | 488 | OG | SER | A | 325 | 27.183 | 35.239 | 14.615 | 1.00 | 48.71 | 8 |
| | ATOM | 489 | C | SER | A | 325 | 27.651 | 38.093 | 13.659 | 1.00 | 50.61 | 6 |
| | ATOM | 490 | O | SER | A | 325 | 26.885 | 38.992 | 13.354 | 1.00 | 52.19 | 8 |
| 45 | ATOM | 491 | N | GLU | A | 326 | 28.495 | 38.168 | 14.687 | 1.00 | 45.64 | 7 |
| | ATOM | 492 | CA | GLU | A | 326 | 28.567 | 39.341 | 15.546 | 1.00 | 43.35 | 6 |
| | ATOM | 493 | CB | GLU | A | 326 | 28.830 | 40.608 | 14.711 | 1.00 | 42.74 | 6 |
| | ATOM | 494 | CG | GLU | A | 326 | 30.148 | 40.606 | 13.945 | 1.00 | 50.32 | 6 |
| | ATOM | 495 | CD | GLU | A | 326 | 30.451 | 41.925 | 13.313 | 1.00 | 56.34 | 6 |
| 50 | ATOM | 496 | OE1 | GLU | A | 326 | 31.509 | 42.046 | 12.649 | 1.00 | 59.31 | 8 |
| | ATOM | 497 | OE2 | GLU | A | 326 | 29.656 | 42.890 | 13.452 | 1.00 | 55.74 | 8 |
| | ATOM | 498 | C | GLU | A | 326 | 27.288 | 39.526 | 16.340 | 1.00 | 40.23 | 6 |
| | ATOM | 499 | O | GLU | A | 326 | 26.695 | 40.603 | 16.340 | 1.00 | 40.44 | 8 |
| | ATOM | 500 | N | THR | A | 327 | 26.888 | 38.474 | 17.051 | 1.00 | 35.90 | 7 |
| 55 | ATOM | 501 | CA | THR | A | 327 | 25.663 | 38.506 | 17.860 | 1.00 | 37.29 | 6 |
| | ATOM | 502 | CB | THR | A | 327 | 24.466 | 38.057 | 17.024 | 1.00 | 37.63 | 6 |
| | ATOM | 503 | OG1 | THR | A | 327 | 24.661 | 36.709 | 16.580 | 1.00 | 38.12 | 8 |
| | ATOM | 504 | CG2 | THR | A | 327 | 24.269 | 38.965 | 15.810 | 1.00 | 39.90 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| 5 | ATOM | 505 | C | THR | A | 327 | 25.767 | 37.562 | 19.038 | 1.00 | 39.49 | 6 |
| | ATOM | 506 | O | THR | A | 327 | 26.284 | 36.458 | 18.903 | 1.00 | 40.50 | 8 |
| | ATOM | 507 | N | LEU | A | 328 | 25.250 | 37.987 | 20.184 | 1.00 | 36.64 | 7 |
| | ATOM | 508 | CA | LEU | A | 328 | 25.264 | 37.141 | 21.381 | 1.00 | 37.73 | 6 |
| | ATOM | 509 | CB | LEU | A | 328 | 25.148 | 37.999 | 22.650 | 1.00 | 37.78 | 6 |
| 10 | ATOM | 510 | CG | LEU | A | 328 | 26.102 | 39.150 | 22.843 | 1.00 | 36.26 | 6 |
| | ATOM | 511 | CD1 | LEU | A | 328 | 26.066 | 39.623 | 24.272 | 1.00 | 36.56 | 6 |
| | ATOM | 512 | CD2 | LEU | A | 328 | 27.481 | 38.688 | 22.500 | 1.00 | 39.85 | 6 |
| | ATOM | 513 | C | LEU | A | 328 | 24.063 | 36.220 | 21.244 | 1.00 | 37.27 | 6 |
| | ATOM | 514 | O | LEU | A | 328 | 23.306 | 36.337 | 20.279 | 1.00 | 34.96 | 8 |
| 15 | ATOM | 515 | N | THR | A | 329 | 23.891 | 35.317 | 22.205 | 1.00 | 39.73 | 7 |
| | ATOM | 516 | CA | THR | A | 329 | 22.785 | 34.376 | 22.180 | 1.00 | 40.81 | 6 |
| | ATOM | 517 | CB | THR | A | 329 | 23.241 | 32.991 | 21.699 | 1.00 | 42.67 | 6 |
| | ATOM | 518 | OG1 | THR | A | 329 | 23.879 | 33.103 | 20.421 | 1.00 | 42.52 | 8 |
| | ATOM | 519 | CG2 | THR | A | 329 | 22.026 | 32.057 | 21.589 | 1.00 | 43.52 | 6 |
| 20 | ATOM | 520 | C | THR | A | 329 | 22.168 | 34.245 | 23.548 | 1.00 | 44.31 | 6 |
| | ATOM | 521 | O | THR | A | 329 | 22.526 | 33.370 | 24.320 | 1.00 | 43.72 | 8 |
| | ATOM | 522 | N | LEU | A | 330 | 21.237 | 35.149 | 23.830 | 1.00 | 44.62 | 7 |
| | ATOM | 523 | CA | LEU | A | 330 | 20.532 | 35.170 | 25.111 | 1.00 | 45.09 | 6 |
| | ATOM | 524 | CB | LEU | A | 330 | 19.677 | 36.444 | 25.195 | 1.00 | 44.66 | 6 |
| 25 | ATOM | 525 | CG | LEU | A | 330 | 20.436 | 37.750 | 25.259 | 1.00 | 51.06 | 6 |
| | ATOM | 526 | CD1 | LEU | A | 330 | 21.405 | 37.831 | 24.104 | 1.00 | 48.58 | 6 |
| | ATOM | 527 | CD2 | LEU | A | 330 | 19.466 | 38.909 | 25.238 | 1.00 | 45.18 | 6 |
| | ATOM | 528 | C | LEU | A | 330 | 19.656 | 33.919 | 25.301 | 1.00 | 48.06 | 6 |
| | ATOM | 529 | O | LEU | A | 330 | 19.049 | 33.422 | 24.359 | 1.00 | 49.33 | 8 |
| 30 | ATOM | 530 | N | ASN | A | 331 | 19.618 | 33.431 | 26.540 | 1.00 | 52.20 | 7 |
| | ATOM | 531 | CA | ASN | A | 331 | 18.842 | 32.256 | 26.913 | 1.00 | 54.41 | 6 |
| | ATOM | 532 | CB | ASN | A | 331 | 17.361 | 32.628 | 27.009 | 1.00 | 54.94 | 6 |
| | ATOM | 533 | CG | ASN | A | 331 | 16.724 | 32.112 | 28.269 | 1.00 | 60.35 | 6 |
| | ATOM | 534 | OD1 | ASN | A | 331 | 17.124 | 32.505 | 29.383 | 1.00 | 61.84 | 8 |
| 35 | ATOM | 535 | ND2 | ASN | A | 331 | 15.750 | 31.238 | 28.117 | 1.00 | 65.92 | 7 |
| | ATOM | 536 | C | ASN | A | 331 | 19.016 | 31.108 | 25.934 | 1.00 | 58.00 | 6 |
| | ATOM | 537 | O | ASN | A | 331 | 18.243 | 30.157 | 25.941 | 1.00 | 60.17 | 8 |
| | ATOM | 538 | N | GLY | A | 332 | 20.063 | 31.196 | 25.114 | 1.00 | 58.45 | 7 |
| | ATOM | 539 | CA | GLY | A | 332 | 20.341 | 30.161 | 24.131 | 1.00 | 58.55 | 6 |
| 40 | ATOM | 540 | C | GLY | A | 332 | 19.316 | 30.016 | 23.021 | 1.00 | 59.79 | 6 |
| | ATOM | 541 | O | GLY | A | 332 | 19.413 | 29.094 | 22.213 | 1.00 | 61.32 | 8 |
| | ATOM | 542 | N | GLU | A | 333 | 18.346 | 30.929 | 22.983 | 1.00 | 60.28 | 7 |
| | ATOM | 543 | CA | GLU | A | 333 | 17.294 | 30.883 | 21.985 | 1.00 | 59.13 | 6 |
| | ATOM | 544 | CB | GLU | A | 333 | 15.919 | 30.875 | 22.662 | 1.00 | 62.40 | 6 |
| 45 | ATOM | 545 | CG | GLU | A | 333 | 15.667 | 29.750 | 23.658 | 1.00 | 75.69 | 6 |
| | ATOM | 546 | CD | GLU | A | 333 | 14.341 | 29.865 | 24.346 | 1.00 | 80.41 | 6 |
| | ATOM | 547 | OE1 | GLU | A | 333 | 14.052 | 30.932 | 24.945 | 1.00 | 79.98 | 8 |
| | ATOM | 548 | OE2 | GLU | A | 333 | 13.549 | 28.884 | 24.329 | 1.00 | 83.81 | 8 |
| | ATOM | 549 | C | GLU | A | 333 | 17.356 | 32.090 | 21.073 | 1.00 | 57.18 | 6 |
| 50 | ATOM | 550 | O | GLU | A | 333 | 17.239 | 31.969 | 19.852 | 1.00 | 57.50 | 8 |
| | ATOM | 551 | N | MET | A | 334 | 17.512 | 33.258 | 21.696 | 1.00 | 55.20 | 7 |
| | ATOM | 552 | CA | MET | A | 334 | 17.561 | 34.529 | 20.980 | 1.00 | 50.85 | 6 |
| | ATOM | 553 | CB | MET | A | 334 | 16.751 | 35.556 | 21.763 | 1.00 | 48.70 | 6 |
| | ATOM | 554 | CG | MET | A | 334 | 16.859 | 36.947 | 21.212 | 1.00 | 45.39 | 6 |
| 55 | ATOM | 555 | SD | MET | A | 334 | 15.881 | 38.186 | 22.127 | 1.00 | 44.56 | 16 |
| | ATOM | 556 | CE | MET | A | 334 | 14.229 | 37.371 | 22.113 | 1.00 | 45.25 | 6 |
| | ATOM | 557 | C | MET | A | 334 | 18.956 | 35.087 | 20.713 | 1.00 | 51.59 | 6 |
| | ATOM | 558 | O | MET | A | 334 | 19.739 | 35.268 | 21.633 | 1.00 | 52.52 | 8 |

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|----|------|-----|-----|-----------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 559 | N | ALA A 335 | 19.234 | 35.371 | 19.444 | 1.00 | 51.00 | 7 |
| | ATOM | 560 | CA | ALA A 335 | 20.520 | 35.932 | 19.039 | 1.00 | 48.98 | 6 |
| | ATOM | 561 | CB | ALA A 335 | 20.997 | 35.254 | 17.768 | 1.00 | 47.86 | 6 |
| | ATOM | 562 | C | ALA A 335 | 20.342 | 37.420 | 18.805 | 1.00 | 51.01 | 6 |
| | ATOM | 563 | O | ALA A 335 | 19.594 | 37.830 | 17.919 | 1.00 | 51.61 | 8 |
| 10 | ATOM | 564 | N | VAL A 336 | 21.024 | 38.232 | 19.612 | 1.00 | 46.62 | 7 |
| | ATOM | 565 | CA | VAL A 336 | 20.910 | 39.699 | 19.502 | 1.00 | 42.35 | 6 |
| | ATOM | 566 | CB | VAL A 336 | 20.517 | 40.325 | 20.840 | 1.00 | 42.41 | 6 |
| | ATOM | 567 | CG1 | VAL A 336 | 19.242 | 39.691 | 21.361 | 1.00 | 42.00 | 6 |
| | ATOM | 568 | CG2 | VAL A 336 | 21.639 | 40.211 | 21.852 | 1.00 | 40.32 | 6 |
| 15 | ATOM | 569 | C | VAL A 336 | 22.204 | 40.321 | 19.036 | 1.00 | 45.33 | 6 |
| | ATOM | 570 | O | VAL A 336 | 23.263 | 39.691 | 19.025 | 1.00 | 47.42 | 8 |
| | ATOM | 571 | N | THR A 337 | 22.090 | 41.590 | 18.668 | 1.00 | 41.60 | 7 |
| | ATOM | 572 | CA | THR A 337 | 23.230 | 42.377 | 18.175 | 1.00 | 39.69 | 6 |
| | ATOM | 573 | CB | THR A 337 | 22.882 | 43.061 | 16.852 | 1.00 | 41.35 | 6 |
| 20 | ATOM | 574 | OG1 | THR A 337 | 21.987 | 44.157 | 17.080 | 1.00 | 49.35 | 8 |
| | ATOM | 575 | CG2 | THR A 337 | 22.216 | 42.067 | 15.904 | 1.00 | 40.38 | 6 |
| | ATOM | 576 | C | THR A 337 | 23.588 | 43.481 | 19.159 | 1.00 | 37.88 | 6 |
| | ATOM | 577 | O | THR A 337 | 22.734 | 43.989 | 19.892 | 1.00 | 34.06 | 8 |
| | ATOM | 578 | N | ARG A 338 | 24.865 | 43.849 | 19.138 | 1.00 | 37.61 | 7 |
| 25 | ATOM | 579 | CA | ARG A 338 | 25.388 | 44.919 | 19.984 | 1.00 | 38.68 | 6 |
| | ATOM | 580 | CB | ARG A 338 | 26.669 | 45.479 | 19.351 | 1.00 | 35.95 | 6 |
| | ATOM | 581 | CG | ARG A 338 | 27.250 | 46.713 | 20.038 | 1.00 | 38.83 | 6 |
| | ATOM | 582 | CD | ARG A 338 | 28.443 | 47.254 | 19.247 | 1.00 | 35.88 | 6 |
| | ATOM | 583 | NE | ARG A 338 | 29.559 | 46.320 | 19.175 | 1.00 | 37.42 | 7 |
| 30 | ATOM | 584 | CZ | ARG A 338 | 30.449 | 46.122 | 20.145 | 1.00 | 30.20 | 6 |
| | ATOM | 585 | NH1 | ARG A 338 | 30.338 | 46.791 | 21.295 | 1.00 | 27.98 | 7 |
| | ATOM | 586 | NH2 | ARG A 338 | 31.433 | 45.240 | 19.954 | 1.00 | 27.40 | 7 |
| | ATOM | 587 | C | ARG A 338 | 24.333 | 46.010 | 20.085 | 1.00 | 38.09 | 6 |
| | ATOM | 588 | O | ARG A 338 | 23.894 | 46.397 | 21.169 | 1.00 | 34.12 | 8 |
| 35 | ATOM | 589 | N | GLY A 339 | 23.915 | 46.496 | 18.922 | 1.00 | 41.25 | 7 |
| | ATOM | 590 | CA | GLY A 339 | 22.918 | 47.547 | 18.890 | 1.00 | 41.35 | 6 |
| | ATOM | 591 | C | GLY A 339 | 21.692 | 47.140 | 19.672 | 1.00 | 41.23 | 6 |
| | ATOM | 592 | O | GLY A 339 | 21.445 | 47.671 | 20.750 | 1.00 | 38.30 | 8 |
| | ATOM | 593 | N | GLN A 340 | 20.924 | 46.203 | 19.105 | 1.00 | 38.58 | 7 |
| 40 | ATOM | 594 | CA | GLN A 340 | 19.701 | 45.700 | 19.729 | 1.00 | 40.79 | 6 |
| | ATOM | 595 | CB | GLN A 340 | 19.436 | 44.260 | 19.253 | 1.00 | 40.82 | 6 |
| | ATOM | 596 | CG | GLN A 340 | 19.087 | 44.146 | 17.767 | 1.00 | 41.10 | 6 |
| | ATOM | 597 | CD | GLN A 340 | 18.876 | 42.705 | 17.305 | 1.00 | 48.84 | 6 |
| | ATOM | 598 | OE1 | GLN A 340 | 19.826 | 41.888 | 17.309 | 1.00 | 50.53 | 8 |
| 45 | ATOM | 599 | NE2 | GLN A 340 | 17.650 | 42.393 | 16.907 | 1.00 | 54.25 | 7 |
| | ATOM | 600 | C | GLN A 340 | 19.779 | 45.750 | 21.263 | 1.00 | 41.50 | 6 |
| | ATOM | 601 | O | GLN A 340 | 18.998 | 46.444 | 21.923 | 1.00 | 42.72 | 8 |
| | ATOM | 602 | N | LEU A 341 | 20.758 | 45.026 | 21.806 | 1.00 | 42.00 | 7 |
| | ATOM | 603 | CA | LEU A 341 | 20.952 | 44.947 | 23.243 | 1.00 | 38.10 | 6 |
| 50 | ATOM | 604 | CB | LEU A 341 | 22.209 | 44.145 | 23.575 | 1.00 | 36.66 | 6 |
| | ATOM | 605 | CG | LEU A 341 | 22.361 | 43.804 | 25.029 | 1.00 | 39.94 | 6 |
| | ATOM | 606 | CD1 | LEU A 341 | 21.219 | 42.884 | 25.410 | 1.00 | 34.98 | 6 |
| | ATOM | 607 | CD2 | LEU A 341 | 23.685 | 43.128 | 25.284 | 1.00 | 40.95 | 6 |
| | ATOM | 608 | C | LEU A 341 | 21.072 | 46.321 | 23.860 | 1.00 | 36.37 | 6 |
| 55 | ATOM | 609 | O | LEU A 341 | 20.484 | 46.588 | 24.892 | 1.00 | 37.89 | 8 |
| | ATOM | 610 | N | LYS A 342 | 21.848 | 47.184 | 23.209 | 1.00 | 33.29 | 7 |
| | ATOM | 611 | CA | LYS A 342 | 22.089 | 48.546 | 23.679 | 1.00 | 35.17 | 6 |
| | ATOM | 612 | CB | LYS A 342 | 23.057 | 49.242 | 22.721 | 1.00 | 34.97 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 613 | CG | LYS | A | 342 | 23.655 | 50.536 | 23.240 | 1.00 | 40.00 | 6 |
| | ATOM | 614 | CD | LYS | A | 342 | 24.673 | 51.109 | 22.245 | 1.00 | 34.48 | 6 |
| | ATOM | 615 | CE | LYS | A | 342 | 25.514 | 52.229 | 22.873 | 1.00 | 37.54 | 6 |
| | ATOM | 616 | NZ | LYS | A | 342 | 26.655 | 52.634 | 21.987 | 1.00 | 42.32 | 7 |
| | ATOM | 617 | C | LYS | A | 342 | 20.796 | 49.349 | 23.774 | 1.00 | 38.29 | 8 |
| 10 | ATOM | 618 | O | LYS | A | 342 | 20.345 | 49.711 | 24.861 | 1.00 | 36.23 | 8 |
| | ATOM | 619 | N | ASN | A | 343 | 20.223 | 49.622 | 22.603 | 1.00 | 39.25 | 7 |
| | ATOM | 620 | CA | ASN | A | 343 | 18.993 | 50.385 | 22.485 | 1.00 | 40.19 | 6 |
| | ATOM | 621 | CB | ASN | A | 343 | 18.521 | 50.373 | 21.033 | 1.00 | 37.96 | 6 |
| | ATOM | 622 | CG | ASN | A | 343 | 19.664 | 50.550 | 20.052 | 1.00 | 39.22 | 6 |
| 15 | ATOM | 623 | OD1 | ASN | A | 343 | 20.428 | 51.537 | 20.125 | 1.00 | 42.37 | 8 |
| | ATOM | 624 | ND2 | ASN | A | 343 | 19.773 | 49.612 | 19.125 | 1.00 | 42.19 | 7 |
| | ATOM | 625 | C | ASN | A | 343 | 17.928 | 49.748 | 23.375 | 1.00 | 40.12 | 6 |
| | ATOM | 626 | O | ASN | A | 343 | 17.010 | 50.417 | 23.859 | 1.00 | 36.01 | 8 |
| | ATOM | 627 | N | GLY | A | 344 | 18.073 | 48.433 | 23.568 | 1.00 | 40.95 | 7 |
| 20 | ATOM | 628 | CA | GLY | A | 344 | 17.152 | 47.670 | 24.394 | 1.00 | 39.25 | 6 |
| | ATOM | 629 | C | GLY | A | 344 | 17.039 | 48.092 | 25.842 | 1.00 | 38.26 | 6 |
| | ATOM | 630 | O | GLY | A | 344 | 16.072 | 47.724 | 26.512 | 1.00 | 35.69 | 8 |
| | ATOM | 631 | N | GLY | A | 345 | 18.017 | 48.857 | 26.329 | 1.00 | 35.89 | 7 |
| | ATOM | 632 | CA | GLY | A | 345 | 17.964 | 49.301 | 27.706 | 1.00 | 34.00 | 6 |
| 25 | ATOM | 633 | C | GLY | A | 345 | 19.273 | 49.199 | 28.443 | 1.00 | 38.64 | 6 |
| | ATOM | 634 | O | GLY | A | 345 | 19.469 | 49.888 | 29.441 | 1.00 | 38.14 | 8 |
| | ATOM | 635 | N | LEU | A | 346 | 20.170 | 48.337 | 27.973 | 1.00 | 39.52 | 7 |
| | ATOM | 636 | CA | LEU | A | 346 | 21.444 | 48.180 | 28.649 | 1.00 | 36.05 | 6 |
| | ATOM | 637 | CB | LEU | A | 346 | 22.124 | 46.876 | 28.209 | 1.00 | 35.72 | 6 |
| 30 | ATOM | 638 | CG | LEU | A | 346 | 21.355 | 45.617 | 28.501 | 1.00 | 34.89 | 6 |
| | ATOM | 639 | CD1 | LEU | A | 346 | 22.295 | 44.413 | 28.422 | 1.00 | 44.09 | 6 |
| | ATOM | 640 | CD2 | LEU | A | 346 | 20.786 | 45.721 | 29.902 | 1.00 | 34.84 | 6 |
| | ATOM | 641 | C | LEU | A | 346 | 22.358 | 49.361 | 28.396 | 1.00 | 33.52 | 6 |
| | ATOM | 642 | O | LEU | A | 346 | 23.267 | 49.653 | 29.178 | 1.00 | 35.58 | 8 |
| 35 | ATOM | 643 | N | GLY | A | 347 | 22.087 | 50.056 | 27.295 | 1.00 | 30.47 | 7 |
| | ATOM | 644 | CA | GLY | A | 347 | 22.909 | 51.192 | 26.931 | 1.00 | 33.01 | 6 |
| | ATOM | 645 | C | GLY | A | 347 | 24.360 | 50.768 | 26.747 | 1.00 | 30.72 | 6 |
| | ATOM | 646 | O | GLY | A | 347 | 24.669 | 49.775 | 26.082 | 1.00 | 30.89 | 8 |
| | ATOM | 647 | N | VAL | A | 348 | 25.244 | 51.556 | 27.355 | 1.00 | 31.30 | 7 |
| 40 | ATOM | 648 | CA | VAL | A | 348 | 26.671 | 51.325 | 27.286 | 1.00 | 31.27 | 6 |
| | ATOM | 649 | CB | VAL | A | 348 | 27.441 | 52.294 | 28.184 | 1.00 | 31.66 | 6 |
| | ATOM | 650 | CG1 | VAL | A | 348 | 27.067 | 52.107 | 29.631 | 1.00 | 20.19 | 6 |
| | ATOM | 651 | CG2 | VAL | A | 348 | 28.931 | 52.138 | 27.986 | 1.00 | 24.77 | 6 |
| | ATOM | 652 | C | VAL | A | 348 | 27.063 | 49.892 | 27.678 | 1.00 | 33.84 | 6 |
| 45 | ATOM | 653 | O | VAL | A | 348 | 28.095 | 49.392 | 27.225 | 1.00 | 29.99 | 8 |
| | ATOM | 654 | N | VAL | A | 349 | 26.253 | 49.227 | 28.514 | 1.00 | 33.31 | 7 |
| | ATOM | 655 | CA | VAL | A | 349 | 26.568 | 47.881 | 28.906 | 1.00 | 32.23 | 6 |
| | ATOM | 656 | CB | VAL | A | 349 | 25.581 | 47.259 | 29.858 | 1.00 | 32.59 | 6 |
| | ATOM | 657 | CG1 | VAL | A | 349 | 25.865 | 45.795 | 29.985 | 1.00 | 33.68 | 6 |
| 50 | ATOM | 658 | CG2 | VAL | A | 349 | 25.687 | 47.899 | 31.213 | 1.00 | 32.30 | 6 |
| | ATOM | 659 | C | VAL | A | 349 | 26.706 | 46.985 | 27.726 | 1.00 | 34.91 | 6 |
| | ATOM | 660 | O | VAL | A | 349 | 27.583 | 46.136 | 27.735 | 1.00 | 33.73 | 8 |
| | ATOM | 661 | N | SER | A | 350 | 25.875 | 47.134 | 26.702 | 1.00 | 32.81 | 7 |
| | ATOM | 662 | CA | SER | A | 350 | 26.001 | 46.252 | 25.556 | 1.00 | 30.10 | 6 |
| 55 | ATOM | 663 | CB | SER | A | 350 | 25.119 | 46.665 | 24.411 | 1.00 | 24.95 | 6 |
| | ATOM | 664 | OG | SER | A | 350 | 25.209 | 45.675 | 23.394 | 1.00 | 23.16 | 8 |
| | ATOM | 665 | C | SER | A | 350 | 27.445 | 46.257 | 25.129 | 1.00 | 31.59 | 6 |
| | ATOM | 666 | O | SER | A | 350 | 28.116 | 45.244 | 25.284 | 1.00 | 37.62 | 8 |

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|----|------|-----|-----|-----------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 667 | N | ASP A 351 | 27.945 | 47.367 | 24.591 | 1.00 | 28.60 | 7 |
| | ATOM | 668 | CA | ASP A 351 | 29.351 | 47.437 | 24.183 | 1.00 | 29.82 | 6 |
| | ATOM | 669 | CB | ASP A 351 | 29.808 | 48.891 | 24.105 | 1.00 | 27.49 | 6 |
| | ATOM | 670 | CG | ASP A 351 | 28.875 | 49.744 | 23.303 | 1.00 | 30.22 | 6 |
| | ATOM | 671 | OD1 | ASP A 351 | 28.055 | 50.483 | 23.909 | 1.00 | 32.61 | 8 |
| 10 | ATOM | 672 | OD2 | ASP A 351 | 28.942 | 49.714 | 22.044 | 1.00 | 30.02 | 8 |
| | ATOM | 673 | C | ASP A 351 | 30.173 | 46.653 | 25.231 | 1.00 | 30.63 | 6 |
| | ATOM | 674 | O | ASP A 351 | 30.981 | 45.792 | 24.903 | 1.00 | 29.54 | 8 |
| | ATOM | 675 | N | ALA A 352 | 29.939 | 46.949 | 26.503 | 1.00 | 25.33 | 7 |
| | ATOM | 676 | CA | ALA A 352 | 30.623 | 46.280 | 27.602 | 1.00 | 28.59 | 6 |
| 15 | ATOM | 677 | CB | ALA A 352 | 30.072 | 46.799 | 28.922 | 1.00 | 20.95 | 6 |
| | ATOM | 678 | C | ALA A 352 | 30.492 | 44.756 | 27.527 | 1.00 | 29.69 | 6 |
| | ATOM | 679 | O | ALA A 352 | 31.481 | 44.054 | 27.587 | 1.00 | 30.36 | 8 |
| | ATOM | 680 | N | ILE A 353 | 29.260 | 44.260 | 27.413 | 1.00 | 27.63 | 7 |
| | ATOM | 681 | CA | ILE A 353 | 29.003 | 42.832 | 27.326 | 1.00 | 27.55 | 6 |
| 20 | ATOM | 682 | CB | ILE A 353 | 27.512 | 42.528 | 27.429 | 1.00 | 28.04 | 6 |
| | ATOM | 683 | CG2 | ILE A 353 | 27.269 | 41.042 | 27.289 | 1.00 | 23.68 | 6 |
| | ATOM | 684 | CG1 | ILE A 353 | 26.955 | 42.965 | 28.789 | 1.00 | 27.33 | 6 |
| | ATOM | 685 | CD1 | ILE A 353 | 25.452 | 42.688 | 28.944 | 1.00 | 26.23 | 6 |
| | ATOM | 686 | C | ILE A 353 | 29.534 | 42.207 | 26.054 | 1.00 | 30.88 | 6 |
| 25 | ATOM | 687 | O | ILE A 353 | 30.007 | 41.076 | 26.068 | 1.00 | 31.22 | 8 |
| | ATOM | 688 | N | PHE A 354 | 29.426 | 42.917 | 24.939 | 1.00 | 29.86 | 7 |
| | ATOM | 689 | CA | PHE A 354 | 29.922 | 42.369 | 23.686 | 1.00 | 31.08 | 6 |
| | ATOM | 690 | CB | PHE A 354 | 29.371 | 43.146 | 22.487 | 1.00 | 28.80 | 6 |
| | ATOM | 691 | CG | PHE A 354 | 28.029 | 42.643 | 21.988 | 1.00 | 28.80 | 6 |
| 30 | ATOM | 692 | CD1 | PHE A 354 | 26.872 | 42.842 | 22.724 | 1.00 | 30.96 | 6 |
| | ATOM | 693 | CD2 | PHE A 354 | 27.950 | 41.953 | 20.783 | 1.00 | 29.45 | 6 |
| | ATOM | 694 | CE1 | PHE A 354 | 25.657 | 42.360 | 22.250 | 1.00 | 27.12 | 6 |
| | ATOM | 695 | CE2 | PHE A 354 | 26.738 | 41.470 | 20.305 | 1.00 | 25.19 | 6 |
| | ATOM | 696 | CZ | PHE A 354 | 25.590 | 41.672 | 21.038 | 1.00 | 28.09 | 6 |
| 35 | ATOM | 697 | C | PHE A 354 | 31.444 | 42.399 | 23.682 | 1.00 | 29.17 | 6 |
| | ATOM | 698 | O | PHE A 354 | 32.087 | 41.389 | 23.398 | 1.00 | 32.62 | 8 |
| | ATOM | 699 | N | ASP A 355 | 32.013 | 43.569 | 23.980 | 1.00 | 23.86 | 7 |
| | ATOM | 700 | CA | ASP A 355 | 33.466 | 43.739 | 24.030 | 1.00 | 25.34 | 6 |
| | ATOM | 701 | CB | ASP A 355 | 33.820 | 45.053 | 24.737 | 1.00 | 21.41 | 6 |
| 40 | ATOM | 702 | CG | ASP A 355 | 33.841 | 46.226 | 23.809 | 1.00 | 32.08 | 6 |
| | ATOM | 703 | OD1 | ASP A 355 | 32.979 | 46.322 | 22.902 | 1.00 | 33.58 | 8 |
| | ATOM | 704 | OD2 | ASP A 355 | 34.711 | 47.117 | 23.968 | 1.00 | 33.20 | 8 |
| | ATOM | 705 | C | ASP A 355 | 34.074 | 42.559 | 24.781 | 1.00 | 27.86 | 6 |
| | ATOM | 706 | O | ASP A 355 | 35.131 | 42.053 | 24.410 | 1.00 | 32.42 | 8 |
| 45 | ATOM | 707 | N | LEU A 356 | 33.387 | 42.128 | 25.843 | 1.00 | 26.84 | 7 |
| | ATOM | 708 | CA | LEU A 356 | 33.845 | 40.993 | 26.642 | 1.00 | 28.66 | 6 |
| | ATOM | 709 | CB | LEU A 356 | 32.893 | 40.747 | 27.825 | 1.00 | 25.37 | 6 |
| | ATOM | 710 | CG | LEU A 356 | 33.235 | 39.608 | 28.755 | 1.00 | 27.61 | 6 |
| | ATOM | 711 | CD1 | LEU A 356 | 34.538 | 39.917 | 29.451 | 1.00 | 25.43 | 6 |
| 50 | ATOM | 712 | CD2 | LEU A 356 | 32.149 | 39.414 | 29.765 | 1.00 | 27.49 | 6 |
| | ATOM | 713 | C | LEU A 356 | 33.849 | 39.779 | 25.723 | 1.00 | 30.44 | 6 |
| | ATOM | 714 | O | LEU A 356 | 34.884 | 39.160 | 25.470 | 1.00 | 31.55 | 8 |
| | ATOM | 715 | N | GLY A 357 | 32.661 | 39.451 | 25.218 | 1.00 | 32.69 | 7 |
| | ATOM | 716 | CA | GLY A 357 | 32.511 | 38.304 | 24.338 | 1.00 | 29.87 | 6 |
| 55 | ATOM | 717 | C | GLY A 357 | 33.653 | 38.157 | 23.359 | 1.00 | 33.12 | 6 |
| | ATOM | 718 | O | GLY A 357 | 34.302 | 37.110 | 23.323 | 1.00 | 29.41 | 8 |
| | ATOM | 719 | N | MET A 358 | 33.876 | 39.206 | 22.564 | 1.00 | 33.31 | 7 |
| | ATOM | 720 | CA | MET A 358 | 34.949 | 39.206 | 21.580 | 1.00 | 35.87 | 6 |

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|----|------|-----|-----|-----------|--------|--------|--------|------|-------|----|
| 5 | ATOM | 721 | CB | MET A 358 | 35.143 | 40.688 | 21.009 | 1.00 | 34.56 | 6 |
| | ATOM | 722 | CG | MET A 358 | 33.949 | 41.145 | 20.290 | 1.00 | 46.43 | 6 |
| | ATOM | 723 | SD | MET A 358 | 34.207 | 42.776 | 19.514 | 1.00 | 42.13 | 16 |
| | ATOM | 724 | CE | MET A 358 | 34.507 | 43.855 | 20.994 | 1.00 | 44.29 | 6 |
| | ATOM | 725 | C | MET A 358 | 36.256 | 38.762 | 22.230 | 1.00 | 33.26 | 6 |
| 10 | ATOM | 726 | O | MET A 358 | 36.894 | 37.807 | 21.795 | 1.00 | 36.39 | 8 |
| | ATOM | 727 | N | SER A 359 | 36.637 | 39.491 | 23.281 | 1.00 | 33.31 | 7 |
| | ATOM | 728 | CA | SER A 359 | 37.860 | 39.226 | 24.019 | 1.00 | 34.39 | 6 |
| | ATOM | 729 | CB | SER A 359 | 37.869 | 40.067 | 25.295 | 1.00 | 30.84 | 6 |
| | ATOM | 730 | OG | SER A 359 | 39.135 | 40.008 | 25.930 | 1.00 | 47.14 | 8 |
| 15 | ATOM | 731 | C | SER A 359 | 37.984 | 37.748 | 24.357 | 1.00 | 36.43 | 6 |
| | ATOM | 732 | O | SER A 359 | 38.900 | 37.078 | 23.896 | 1.00 | 35.46 | 8 |
| | ATOM | 733 | N | LEU A 360 | 37.046 | 37.264 | 25.166 | 1.00 | 36.74 | 7 |
| | ATOM | 734 | CA | LEU A 360 | 37.017 | 35.875 | 25.604 | 1.00 | 35.44 | 6 |
| | ATOM | 735 | CB | LEU A 360 | 35.708 | 35.579 | 26.336 | 1.00 | 34.16 | 6 |
| 20 | ATOM | 736 | CG | LEU A 360 | 35.471 | 36.290 | 27.644 | 1.00 | 34.59 | 6 |
| | ATOM | 737 | CD1 | LEU A 360 | 34.225 | 35.765 | 28.312 | 1.00 | 33.53 | 6 |
| | ATOM | 738 | CD2 | LEU A 360 | 36.658 | 36.052 | 28.541 | 1.00 | 31.69 | 6 |
| | ATOM | 739 | C | LEU A 360 | 37.203 | 34.862 | 24.500 | 1.00 | 38.72 | 6 |
| | ATOM | 740 | O | LEU A 360 | 37.820 | 33.828 | 24.728 | 1.00 | 38.29 | 8 |
| 25 | ATOM | 741 | N | SER A 361 | 36.635 | 35.147 | 23.328 | 1.00 | 40.96 | 7 |
| | ATOM | 742 | CA | SER A 361 | 36.777 | 34.262 | 22.186 | 1.00 | 45.67 | 6 |
| | ATOM | 743 | CB | SER A 361 | 36.518 | 35.045 | 20.904 | 1.00 | 46.45 | 6 |
| | ATOM | 744 | OG | SER A 361 | 35.210 | 35.598 | 20.906 | 1.00 | 51.81 | 8 |
| | ATOM | 745 | C | SER A 361 | 38.166 | 33.627 | 22.145 | 1.00 | 44.49 | 6 |
| 30 | ATOM | 746 | O | SER A 361 | 38.347 | 32.538 | 21.625 | 1.00 | 46.67 | 8 |
| | ATOM | 747 | N | SER A 362 | 39.134 | 34.348 | 22.703 | 1.00 | 41.44 | 7 |
| | ATOM | 748 | CA | SER A 362 | 40.525 | 33.918 | 22.790 | 1.00 | 42.13 | 6 |
| | ATOM | 749 | CB | SER A 362 | 41.408 | 35.131 | 23.066 | 1.00 | 42.61 | 6 |
| | ATOM | 750 | OG | SER A 362 | 41.219 | 36.136 | 22.076 | 1.00 | 51.87 | 8 |
| 35 | ATOM | 751 | C | SER A 362 | 40.798 | 32.870 | 23.876 | 1.00 | 38.41 | 6 |
| | ATOM | 752 | O | SER A 362 | 41.553 | 31.938 | 23.641 | 1.00 | 38.01 | 8 |
| | ATOM | 753 | N | PHE A 363 | 40.198 | 33.039 | 25.058 | 1.00 | 34.55 | 7 |
| | ATOM | 754 | CA | PHE A 363 | 40.417 | 32.126 | 26.174 | 1.00 | 32.96 | 6 |
| | ATOM | 755 | CB | PHE A 363 | 39.832 | 32.718 | 27.447 | 1.00 | 31.99 | 6 |
| 40 | ATOM | 756 | CG | PHE A 363 | 40.448 | 34.036 | 27.840 | 1.00 | 29.97 | 6 |
| | ATOM | 757 | CD1 | PHE A 363 | 40.102 | 34.650 | 29.020 | 1.00 | 30.61 | 6 |
| | ATOM | 758 | CD2 | PHE A 363 | 41.379 | 34.646 | 27.014 | 1.00 | 32.02 | 6 |
| | ATOM | 759 | CE1 | PHE A 363 | 40.685 | 35.856 | 29.391 | 1.00 | 33.67 | 6 |
| | ATOM | 760 | CE2 | PHE A 363 | 41.959 | 35.843 | 27.377 | 1.00 | 30.91 | 6 |
| 45 | ATOM | 761 | CZ | PHE A 363 | 41.615 | 36.456 | 28.558 | 1.00 | 29.33 | 6 |
| | ATOM | 762 | C | PHE A 363 | 39.883 | 30.716 | 25.967 | 1.00 | 30.52 | 6 |
| | ATOM | 763 | O | PHE A 363 | 40.436 | 29.766 | 26.526 | 1.00 | 32.19 | 8 |
| | ATOM | 764 | N | ASN A 364 | 38.817 | 30.570 | 25.175 | 1.00 | 33.51 | 7 |
| | ATOM | 765 | CA | ASN A 364 | 38.239 | 29.264 | 24.918 | 1.00 | 38.03 | 6 |
| 50 | ATOM | 766 | CB | ASN A 364 | 39.240 | 28.404 | 24.139 | 1.00 | 42.32 | 6 |
| | ATOM | 767 | CG | ASN A 364 | 39.696 | 29.065 | 22.861 | 1.00 | 53.11 | 6 |
| | ATOM | 768 | OD1 | ASN A 364 | 38.874 | 29.330 | 21.954 | 1.00 | 59.51 | 8 |
| | ATOM | 769 | ND2 | ASN A 364 | 40.986 | 29.330 | 22.772 | 1.00 | 55.95 | 7 |
| | ATOM | 770 | C | ASN A 364 | 37.916 | 28.572 | 26.235 | 1.00 | 31.89 | 6 |
| 55 | ATOM | 771 | O | ASN A 364 | 38.324 | 27.428 | 26.457 | 1.00 | 30.28 | 8 |
| | ATOM | 772 | N | LEU A 365 | 37.176 | 29.271 | 27.094 | 1.00 | 27.62 | 7 |
| | ATOM | 773 | CA | LEU A 365 | 36.806 | 28.743 | 28.406 | 1.00 | 29.36 | 6 |
| | ATOM | 774 | CB | LEU A 365 | 36.195 | 29.866 | 29.237 | 1.00 | 27.54 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 775 | CG | LEU | A | 365 | 36.990 | 31.150 | 29.185 | 1.00 | 38.91 | 6 |
| | ATOM | 776 | CD1 | LEU | A | 365 | 36.316 | 32.216 | 30.036 | 1.00 | 34.47 | 6 |
| | ATOM | 777 | CD2 | LEU | A | 365 | 38.406 | 30.883 | 29.663 | 1.00 | 34.24 | 6 |
| | ATOM | 778 | C | LEU | A | 365 | 35.830 | 27.590 | 28.262 | 1.00 | 26.23 | 6 |
| | ATOM | 779 | O | LEU | A | 365 | 34.890 | 27.649 | 27.472 | 1.00 | 27.06 | 8 |
| 10 | ATOM | 780 | N | ASP | A | 366 | 36.083 | 26.528 | 29.021 | 1.00 | 25.23 | 7 |
| | ATOM | 781 | CA | ASP | A | 366 | 35.213 | 25.358 | 28.988 | 1.00 | 26.07 | 6 |
| | ATOM | 782 | CB | ASP | A | 366 | 36.027 | 24.049 | 29.033 | 1.00 | 29.68 | 6 |
| | ATOM | 783 | CG | ASP | A | 366 | 36.799 | 23.874 | 30.303 | 1.00 | 35.74 | 6 |
| | ATOM | 784 | OD1 | ASP | A | 366 | 36.285 | 24.177 | 31.402 | 1.00 | 36.78 | 8 |
| 15 | ATOM | 785 | OD2 | ASP | A | 366 | 37.959 | 23.386 | 30.240 | 1.00 | 41.23 | 8 |
| | ATOM | 786 | C | ASP | A | 366 | 34.278 | 25.434 | 30.181 | 1.00 | 27.70 | 6 |
| | ATOM | 787 | O | ASP | A | 366 | 34.587 | 26.097 | 31.173 | 1.00 | 31.94 | 8 |
| | ATOM | 788 | N | ASP | A | 367 | 33.141 | 24.743 | 30.066 | 1.00 | 29.18 | 7 |
| | ATOM | 789 | CA | ASP | A | 367 | 32.120 | 24.679 | 31.120 | 1.00 | 32.72 | 6 |
| 20 | ATOM | 790 | CB | ASP | A | 367 | 31.472 | 23.284 | 31.147 | 1.00 | 38.04 | 6 |
| | ATOM | 791 | CG | ASP | A | 367 | 30.806 | 22.924 | 29.854 | 1.00 | 42.43 | 6 |
| | ATOM | 792 | OD1 | ASP | A | 367 | 29.877 | 23.650 | 29.409 | 1.00 | 35.95 | 8 |
| | ATOM | 793 | OD2 | ASP | A | 367 | 31.186 | 21.884 | 29.250 | 1.00 | 51.42 | 8 |
| | ATOM | 794 | C | ASP | A | 367 | 32.754 | 24.969 | 32.482 | 1.00 | 33.71 | 6 |
| 25 | ATOM | 795 | O | ASP | A | 367 | 32.484 | 26.000 | 33.098 | 1.00 | 38.30 | 8 |
| | ATOM | 796 | N | THR | A | 368 | 33.602 | 24.032 | 32.919 | 1.00 | 31.06 | 7 |
| | ATOM | 797 | CA | THR | A | 368 | 34.329 | 24.124 | 34.181 | 1.00 | 26.28 | 6 |
| | ATOM | 798 | CB | THR | A | 368 | 35.559 | 23.222 | 34.141 | 1.00 | 27.30 | 6 |
| | ATOM | 799 | OG1 | THR | A | 368 | 35.161 | 21.871 | 33.885 | 1.00 | 33.42 | 8 |
| 30 | ATOM | 800 | CG2 | THR | A | 368 | 36.323 | 23.303 | 35.454 | 1.00 | 25.16 | 6 |
| | ATOM | 801 | C | THR | A | 368 | 34.764 | 25.557 | 34.479 | 1.00 | 21.13 | 6 |
| | ATOM | 802 | O | THR | A | 368 | 34.408 | 26.153 | 35.503 | 1.00 | 23.17 | 8 |
| | ATOM | 803 | N | GLU | A | 369 | 35.545 | 26.092 | 33.551 | 1.00 | 21.32 | 7 |
| | ATOM | 804 | CA | GLU | A | 369 | 36.065 | 27.435 | 33.661 | 1.00 | 28.00 | 6 |
| 35 | ATOM | 805 | CB | GLU | A | 369 | 36.960 | 27.707 | 32.453 | 1.00 | 32.79 | 6 |
| | ATOM | 806 | CG | GLU | A | 369 | 38.089 | 26.663 | 32.346 | 1.00 | 36.29 | 6 |
| | ATOM | 807 | CD | GLU | A | 369 | 38.906 | 26.747 | 31.110 | 1.00 | 41.03 | 6 |
| | ATOM | 808 | OE1 | GLU | A | 369 | 38.337 | 26.744 | 29.994 | 1.00 | 42.05 | 8 |
| | ATOM | 809 | OE2 | GLU | A | 369 | 40.158 | 26.795 | 31.218 | 1.00 | 42.03 | 8 |
| 40 | ATOM | 810 | C | GLU | A | 369 | 34.953 | 28.471 | 33.821 | 1.00 | 25.57 | 6 |
| | ATOM | 811 | O | GLU | A | 369 | 34.987 | 29.256 | 34.760 | 1.00 | 20.56 | 8 |
| | ATOM | 812 | N | VAL | A | 370 | 33.967 | 28.463 | 32.921 | 1.00 | 25.39 | 7 |
| | ATOM | 813 | CA | VAL | A | 370 | 32.849 | 29.396 | 33.029 | 1.00 | 25.99 | 6 |
| | ATOM | 814 | CB | VAL | A | 370 | 31.763 | 29.131 | 31.987 | 1.00 | 26.15 | 6 |
| 45 | ATOM | 815 | CG1 | VAL | A | 370 | 30.609 | 30.093 | 32.183 | 1.00 | 27.65 | 6 |
| | ATOM | 816 | CG2 | VAL | A | 370 | 32.306 | 29.251 | 30.592 | 1.00 | 17.70 | 6 |
| | ATOM | 817 | C | VAL | A | 370 | 32.245 | 29.209 | 34.412 | 1.00 | 26.49 | 6 |
| | ATOM | 818 | O | VAL | A | 370 | 32.012 | 30.170 | 35.147 | 1.00 | 28.16 | 8 |
| | ATOM | 819 | N | ALA | A | 371 | 31.988 | 27.947 | 34.739 | 1.00 | 21.01 | 7 |
| 50 | ATOM | 820 | CA | ALA | A | 371 | 31.393 | 27.554 | 36.011 | 1.00 | 19.57 | 6 |
| | ATOM | 821 | CB | ALA | A | 371 | 31.441 | 26.039 | 36.145 | 1.00 | 18.62 | 6 |
| | ATOM | 822 | C | ALA | A | 371 | 32.116 | 28.211 | 37.177 | 1.00 | 23.48 | 6 |
| | ATOM | 823 | O | ALA | A | 371 | 31.531 | 28.989 | 37.931 | 1.00 | 32.67 | 8 |
| | ATOM | 824 | N | LEU | A | 372 | 33.401 | 27.893 | 37.305 | 1.00 | 22.89 | 7 |
| 55 | ATOM | 825 | CA | LEU | A | 372 | 34.217 | 28.447 | 38.369 | 1.00 | 23.28 | 6 |
| | ATOM | 826 | CB | LEU | A | 372 | 35.675 | 27.996 | 38.178 | 1.00 | 27.76 | 6 |
| | ATOM | 827 | CG | LEU | A | 372 | 35.943 | 26.524 | 38.415 | 1.00 | 21.18 | 6 |
| | ATOM | 828 | CD1 | LEU | A | 372 | 37.356 | 26.171 | 38.049 | 1.00 | 27.64 | 6 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| 5 | ATOM | 829 | CD2 | LEU | A | 372 | 35.675 | 26.204 | 39.880 | 1.00 | 20.90 | 6 |
| | ATOM | 830 | C | LEU | A | 372 | 34.098 | 29.966 | 38.396 | 1.00 | 21.34 | 6 |
| | ATOM | 831 | O | LEU | A | 372 | 33.828 | 30.572 | 39.439 | 1.00 | 23.16 | 8 |
| | ATOM | 832 | N | LEU | A | 373 | 34.288 | 30.561 | 37.223 | 1.00 | 24.42 | 7 |
| | ATOM | 833 | CA | LEU | A | 373 | 34.214 | 32.007 | 37.074 | 1.00 | 23.78 | 6 |
| 10 | ATOM | 834 | CB | LEU | A | 373 | 34.296 | 32.360 | 35.575 | 1.00 | 22.18 | 6 |
| | ATOM | 835 | CG | LEU | A | 373 | 34.784 | 33.726 | 35.165 | 1.00 | 31.52 | 6 |
| | ATOM | 836 | CD1 | LEU | A | 373 | 36.000 | 34.084 | 35.962 | 1.00 | 31.93 | 6 |
| | ATOM | 837 | CD2 | LEU | A | 373 | 35.103 | 33.720 | 33.693 | 1.00 | 30.24 | 6 |
| | ATOM | 838 | C | LEU | A | 373 | 32.904 | 32.480 | 37.720 | 1.00 | 25.69 | 6 |
| 15 | ATOM | 839 | O | LEU | A | 373 | 32.895 | 33.410 | 38.532 | 1.00 | 30.13 | 8 |
| | ATOM | 840 | N | GLN | A | 374 | 31.814 | 31.800 | 37.368 | 1.00 | 26.24 | 7 |
| | ATOM | 841 | CA | GLN | A | 374 | 30.487 | 32.104 | 37.896 | 1.00 | 21.60 | 6 |
| | ATOM | 842 | CB | GLN | A | 374 | 29.454 | 31.121 | 37.335 | 1.00 | 24.57 | 6 |
| | ATOM | 843 | CG | GLN | A | 374 | 29.310 | 31.145 | 35.821 | 1.00 | 21.02 | 6 |
| 20 | ATOM | 844 | CD | GLN | A | 374 | 28.224 | 30.201 | 35.331 | 1.00 | 22.86 | 6 |
| | ATOM | 845 | OE1 | GLN | A | 374 | 28.037 | 30.042 | 34.123 | 1.00 | 24.07 | 8 |
| | ATOM | 846 | NE2 | GLN | A | 374 | 27.515 | 29.590 | 36.249 | 1.00 | 25.59 | 7 |
| | ATOM | 847 | C | GLN | A | 374 | 30.421 | 32.039 | 39.422 | 1.00 | 20.66 | 6 |
| | ATOM | 848 | O | GLN | A | 374 | 29.717 | 32.832 | 40.048 | 1.00 | 24.47 | 8 |
| 25 | ATOM | 849 | N | ALA | A | 375 | 31.136 | 31.074 | 40.004 | 1.00 | 16.26 | 7 |
| | ATOM | 850 | CA | ALA | A | 375 | 31.155 | 30.889 | 41.445 | 1.00 | 17.16 | 6 |
| | ATOM | 851 | CB | ALA | A | 375 | 31.805 | 29.568 | 41.780 | 1.00 | 19.53 | 6 |
| | ATOM | 852 | C | ALA | A | 375 | 31.907 | 32.025 | 42.108 | 1.00 | 25.13 | 6 |
| | ATOM | 853 | O | ALA | A | 375 | 31.397 | 32.646 | 43.034 | 1.00 | 23.81 | 8 |
| 30 | ATOM | 854 | N | VAL | A | 376 | 33.122 | 32.277 | 41.611 | 1.00 | 24.57 | 7 |
| | ATOM | 855 | CA | VAL | A | 376 | 33.959 | 33.354 | 42.118 | 1.00 | 25.80 | 6 |
| | ATOM | 856 | CB | VAL | A | 376 | 35.101 | 33.658 | 41.164 | 1.00 | 26.48 | 6 |
| | ATOM | 857 | CG1 | VAL | A | 376 | 35.926 | 34.812 | 41.697 | 1.00 | 23.20 | 6 |
| | ATOM | 858 | CG2 | VAL | A | 376 | 35.959 | 32.429 | 40.952 | 1.00 | 19.08 | 6 |
| 35 | ATOM | 859 | C | VAL | A | 376 | 33.107 | 34.599 | 42.312 | 1.00 | 25.69 | 6 |
| | ATOM | 860 | O | VAL | A | 376 | 33.297 | 35.364 | 43.251 | 1.00 | 27.87 | 8 |
| | ATOM | 861 | N | LEU | A | 377 | 32.159 | 34.781 | 41.399 | 1.00 | 23.09 | 7 |
| | ATOM | 862 | CA | LEU | A | 377 | 31.242 | 35.915 | 41.423 | 1.00 | 22.86 | 6 |
| | ATOM | 863 | CB | LEU | A | 377 | 30.540 | 36.031 | 40.061 | 1.00 | 18.50 | 6 |
| 40 | ATOM | 864 | CG | LEU | A | 377 | 31.424 | 36.368 | 38.885 | 1.00 | 22.65 | 6 |
| | ATOM | 865 | CD1 | LEU | A | 377 | 30.689 | 36.227 | 37.601 | 1.00 | 16.70 | 6 |
| | ATOM | 866 | CD2 | LEU | A | 377 | 31.916 | 37.776 | 39.051 | 1.00 | 19.58 | 6 |
| | ATOM | 867 | C | LEU | A | 377 | 30.228 | 35.719 | 42.543 | 1.00 | 26.14 | 6 |
| | ATOM | 868 | O | LEU | A | 377 | 30.131 | 36.532 | 43.452 | 1.00 | 20.62 | 8 |
| 45 | ATOM | 869 | N | LEU | A | 378 | 29.483 | 34.614 | 42.468 | 1.00 | 28.99 | 7 |
| | ATOM | 870 | CA | LEU | A | 378 | 28.469 | 34.303 | 43.475 | 1.00 | 28.87 | 6 |
| | ATOM | 871 | CB | LEU | A | 378 | 28.053 | 32.826 | 43.397 | 1.00 | 26.89 | 6 |
| | ATOM | 872 | CG | LEU | A | 378 | 27.110 | 32.344 | 44.472 | 1.00 | 28.83 | 6 |
| | ATOM | 873 | CD1 | LEU | A | 378 | 25.915 | 33.252 | 44.525 | 1.00 | 27.97 | 6 |
| 50 | ATOM | 874 | CD2 | LEU | A | 378 | 26.693 | 30.928 | 44.205 | 1.00 | 27.69 | 6 |
| | ATOM | 875 | C | LEU | A | 378 | 28.992 | 34.617 | 44.853 | 1.00 | 31.09 | 6 |
| | ATOM | 876 | O | LEU | A | 378 | 28.399 | 35.421 | 45.573 | 1.00 | 31.77 | 8 |
| | ATOM | 877 | N | MET | A | 379 | 30.118 | 33.991 | 45.189 | 1.00 | 31.44 | 7 |
| | ATOM | 878 | CA | MET | A | 379 | 30.736 | 34.141 | 46.494 | 1.00 | 32.62 | 6 |
| 55 | ATOM | 879 | CB | MET | A | 379 | 31.690 | 32.960 | 46.744 | 1.00 | 31.45 | 6 |
| | ATOM | 880 | CG | MET | A | 379 | 30.984 | 31.595 | 46.792 | 1.00 | 38.75 | 6 |
| | ATOM | 881 | SD | MET | A | 379 | 29.741 | 31.626 | 48.107 | 1.00 | 41.27 | 16 |
| | ATOM | 882 | CE | MET | A | 379 | 28.896 | 30.036 | 47.851 | 1.00 | 35.68 | 6 |

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|----|------|-----|-----|-----------|--------|--------|--------|------|-------|---|
| 5 | ATOM | 883 | C | MET A 379 | 31.485 | 35.448 | 46.724 | 1.00 | 33.72 | 6 |
| | ATOM | 884 | O | MET A 379 | 32.567 | 35.450 | 47.305 | 1.00 | 36.29 | 8 |
| | ATOM | 885 | N | SER A 380 | 30.889 | 36.555 | 46.315 | 1.00 | 34.49 | 7 |
| | ATOM | 886 | CA | SER A 380 | 31.498 | 37.853 | 46.550 | 1.00 | 33.97 | 6 |
| | ATOM | 887 | CB | SER A 380 | 30.921 | 38.890 | 45.576 | 1.00 | 31.24 | 6 |
| 10 | ATOM | 888 | OG | SER A 380 | 31.205 | 38.543 | 44.230 | 1.00 | 39.42 | 8 |
| | ATOM | 889 | C | SER A 380 | 31.179 | 38.239 | 47.992 | 1.00 | 39.69 | 6 |
| | ATOM | 890 | O | SER A 380 | 30.029 | 38.446 | 48.357 | 1.00 | 44.64 | 8 |
| | ATOM | 891 | N | SER A 381 | 32.214 | 38.313 | 48.812 | 1.00 | 41.04 | 7 |
| | ATOM | 892 | CA | SER A 381 | 32.060 | 38.640 | 50.216 | 1.00 | 44.91 | 6 |
| 15 | ATOM | 893 | CB | SER A 381 | 33.324 | 38.234 | 50.951 | 1.00 | 44.50 | 6 |
| | ATOM | 894 | OG | SER A 381 | 34.431 | 39.002 | 50.510 | 1.00 | 45.42 | 8 |
| | ATOM | 895 | C | SER A 381 | 31.795 | 40.106 | 50.499 | 1.00 | 44.59 | 6 |
| | ATOM | 896 | O | SER A 381 | 31.476 | 40.470 | 51.618 | 1.00 | 49.32 | 8 |
| | ATOM | 897 | N | ASP A 382 | 31.939 | 40.942 | 49.486 | 1.00 | 43.75 | 7 |
| 20 | ATOM | 898 | CA | ASP A 382 | 31.744 | 42.362 | 49.641 | 1.00 | 43.93 | 6 |
| | ATOM | 899 | CB | ASP A 382 | 32.673 | 43.111 | 48.677 | 1.00 | 48.39 | 6 |
| | ATOM | 900 | CG | ASP A 382 | 32.572 | 42.624 | 47.263 | 1.00 | 53.23 | 6 |
| | ATOM | 901 | OD1 | ASP A 382 | 32.705 | 41.400 | 47.034 | 1.00 | 56.97 | 8 |
| | ATOM | 902 | OD2 | ASP A 382 | 32.358 | 43.454 | 46.333 | 1.00 | 58.91 | 8 |
| 25 | ATOM | 903 | C | ASP A 382 | 30.314 | 42.885 | 49.507 | 1.00 | 41.09 | 6 |
| | ATOM | 904 | O | ASP A 382 | 30.048 | 44.036 | 49.845 | 1.00 | 40.93 | 8 |
| | ATOM | 905 | N | ARG A 383 | 29.397 | 42.049 | 49.034 | 1.00 | 42.63 | 7 |
| | ATOM | 906 | CA | ARG A 383 | 28.036 | 42.485 | 48.876 | 1.00 | 43.32 | 6 |
| | ATOM | 907 | CB | ARG A 383 | 27.138 | 41.332 | 48.443 | 1.00 | 42.31 | 6 |
| 30 | ATOM | 908 | CG | ARG A 383 | 27.651 | 40.399 | 47.352 | 1.00 | 40.83 | 6 |
| | ATOM | 909 | CD | ARG A 383 | 27.586 | 40.954 | 45.925 | 1.00 | 38.09 | 6 |
| | ATOM | 910 | NE | ARG A 383 | 27.768 | 39.878 | 44.975 | 1.00 | 37.33 | 7 |
| | ATOM | 911 | CZ | ARG A 383 | 28.037 | 40.058 | 43.693 | 1.00 | 38.35 | 6 |
| | ATOM | 912 | NH1 | ARG A 383 | 28.142 | 41.292 | 43.198 | 1.00 | 33.70 | 7 |
| 35 | ATOM | 913 | NH2 | ARG A 383 | 28.194 | 38.992 | 42.918 | 1.00 | 35.46 | 7 |
| | ATOM | 914 | C | ARG A 383 | 27.523 | 42.989 | 50.216 | 1.00 | 44.96 | 6 |
| | ATOM | 915 | O | ARG A 383 | 27.744 | 42.344 | 51.260 | 1.00 | 45.60 | 8 |
| | ATOM | 916 | N | PRO A 384 | 26.852 | 44.144 | 50.223 | 1.00 | 45.33 | 7 |
| | ATOM | 917 | CD | PRO A 384 | 26.625 | 44.964 | 49.027 | 1.00 | 46.85 | 6 |
| 40 | ATOM | 918 | CA | PRO A 384 | 26.298 | 44.738 | 51.446 | 1.00 | 47.37 | 6 |
| | ATOM | 919 | CB | PRO A 384 | 25.841 | 46.130 | 51.012 | 1.00 | 46.90 | 6 |
| | ATOM | 920 | CG | PRO A 384 | 26.075 | 46.229 | 49.567 | 1.00 | 46.41 | 6 |
| | ATOM | 921 | C | PRO A 384 | 25.158 | 43.919 | 52.049 | 1.00 | 48.29 | 6 |
| | ATOM | 922 | O | PRO A 384 | 24.404 | 43.264 | 51.329 | 1.00 | 48.34 | 8 |
| 45 | ATOM | 923 | N | GLY A 385 | 25.039 | 43.983 | 53.383 | 1.00 | 49.88 | 7 |
| | ATOM | 924 | CA | GLY A 385 | 23.991 | 43.270 | 54.113 | 1.00 | 50.35 | 6 |
| | ATOM | 925 | C | GLY A 385 | 24.347 | 41.852 | 54.495 | 1.00 | 50.70 | 6 |
| | ATOM | 926 | O | GLY A 385 | 23.614 | 41.204 | 55.244 | 1.00 | 53.48 | 8 |
| | ATOM | 927 | N | LEU A 386 | 25.466 | 41.371 | 53.955 | 1.00 | 49.04 | 7 |
| 50 | ATOM | 928 | CA | LEU A 386 | 25.901 | 40.017 | 54.215 | 1.00 | 50.53 | 6 |
| | ATOM | 929 | CB | LEU A 386 | 27.224 | 39.751 | 53.492 | 1.00 | 45.17 | 6 |
| | ATOM | 930 | CG | LEU A 386 | 27.152 | 39.592 | 51.993 | 1.00 | 48.26 | 6 |
| | ATOM | 931 | CD1 | LEU A 386 | 28.542 | 39.439 | 51.404 | 1.00 | 41.68 | 6 |
| | ATOM | 932 | CD2 | LEU A 386 | 26.302 | 38.374 | 51.682 | 1.00 | 38.40 | 6 |
| 55 | ATOM | 933 | C | LEU A 386 | 26.045 | 39.776 | 55.691 | 1.00 | 52.13 | 6 |
| | ATOM | 934 | O | LEU A 386 | 26.296 | 40.692 | 56.459 | 1.00 | 53.67 | 8 |
| | ATOM | 935 | N | ALA A 387 | 25.861 | 38.522 | 56.077 | 1.00 | 53.42 | 7 |
| | ATOM | 936 | CA | ALA A 387 | 25.976 | 38.129 | 57.470 | 1.00 | 56.01 | 6 |

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|----|------|-----|-----|-------|-----|--------|--------|--------|------|-------|----|
| 5 | ATOM | 937 | CB | ALA A | 387 | 24.802 | 37.234 | 57.854 | 1.00 | 56.47 | 6 |
| | ATOM | 938 | C | ALA A | 387 | 27.289 | 37.385 | 57.659 | 1.00 | 55.52 | 6 |
| | ATOM | 939 | O | ALA A | 387 | 28.275 | 37.940 | 58.134 | 1.00 | 53.75 | 8 |
| | ATOM | 940 | N | CYS A | 388 | 27.273 | 36.120 | 57.253 | 1.00 | 56.03 | 7 |
| | ATOM | 941 | CA | CYS A | 388 | 28.412 | 35.236 | 57.370 | 1.00 | 59.57 | 6 |
| 10 | ATOM | 942 | CB | CYS A | 388 | 27.923 | 33.803 | 57.172 | 1.00 | 59.23 | 6 |
| | ATOM | 943 | SG | CYS A | 388 | 26.397 | 33.431 | 58.009 | 1.00 | 58.64 | 16 |
| | ATOM | 944 | C | CYS A | 388 | 29.482 | 35.581 | 56.328 | 1.00 | 62.18 | 6 |
| | ATOM | 945 | O | CYS A | 388 | 29.720 | 34.821 | 55.400 | 1.00 | 67.88 | 8 |
| | ATOM | 946 | N | VAL A | 389 | 30.110 | 36.747 | 56.495 | 1.00 | 60.78 | 7 |
| 15 | ATOM | 947 | CA | VAL A | 389 | 31.173 | 37.212 | 55.590 | 1.00 | 57.70 | 6 |
| | ATOM | 948 | CB | VAL A | 389 | 31.740 | 38.567 | 56.024 | 1.00 | 57.09 | 6 |
| | ATOM | 949 | CG1 | VAL A | 389 | 32.795 | 39.037 | 55.041 | 1.00 | 59.03 | 6 |
| | ATOM | 950 | CG2 | VAL A | 389 | 30.640 | 39.598 | 56.171 | 1.00 | 53.98 | 6 |
| | ATOM | 951 | C | VAL A | 389 | 32.297 | 36.182 | 55.550 | 1.00 | 57.77 | 6 |
| 20 | ATOM | 952 | O | VAL A | 389 | 32.358 | 35.336 | 54.662 | 1.00 | 60.94 | 8 |
| | ATOM | 953 | N | ALA A | 390 | 33.182 | 36.292 | 56.528 | 1.00 | 52.68 | 7 |
| | ATOM | 954 | CA | ALA A | 390 | 34.347 | 35.431 | 56.684 | 1.00 | 48.41 | 6 |
| | ATOM | 955 | CB | ALA A | 390 | 34.703 | 35.321 | 58.185 | 1.00 | 45.19 | 6 |
| | ATOM | 956 | C | ALA A | 390 | 34.224 | 34.040 | 56.082 | 1.00 | 47.63 | 6 |
| 25 | ATOM | 957 | O | ALA A | 390 | 35.107 | 33.597 | 55.348 | 1.00 | 51.95 | 8 |
| | ATOM | 958 | N | ARG A | 391 | 33.117 | 33.366 | 56.391 | 1.00 | 47.11 | 7 |
| | ATOM | 959 | CA | ARG A | 391 | 32.879 | 32.018 | 55.885 | 1.00 | 51.64 | 6 |
| | ATOM | 960 | CB | ARG A | 391 | 31.520 | 31.498 | 56.383 | 1.00 | 54.22 | 6 |
| | ATOM | 961 | CG | ARG A | 391 | 31.267 | 30.012 | 56.059 | 1.00 | 64.20 | 6 |
| 30 | ATOM | 962 | CD | ARG A | 391 | 29.930 | 29.489 | 56.602 | 1.00 | 73.80 | 6 |
| | ATOM | 963 | NE | ARG A | 391 | 29.787 | 28.044 | 56.454 | 1.00 | 79.76 | 7 |
| | ATOM | 964 | CZ | ARG A | 391 | 30.573 | 27.140 | 57.043 | 1.00 | 84.27 | 6 |
| | ATOM | 965 | NH1 | ARG A | 391 | 31.598 | 27.535 | 57.806 | 1.00 | 85.28 | 7 |
| | ATOM | 966 | NH2 | ARG A | 391 | 30.340 | 25.840 | 56.849 | 1.00 | 86.84 | 7 |
| 35 | ATOM | 967 | C | ARG A | 391 | 32.922 | 31.986 | 54.358 | 1.00 | 48.18 | 6 |
| | ATOM | 968 | O | ARG A | 391 | 33.494 | 31.080 | 53.756 | 1.00 | 49.57 | 8 |
| | ATOM | 969 | N | ILE A | 392 | 32.281 | 32.993 | 53.762 | 1.00 | 45.01 | 7 |
| | ATOM | 970 | CA | ILE A | 392 | 32.196 | 33.148 | 52.319 | 1.00 | 48.77 | 6 |
| | ATOM | 971 | CB | ILE A | 392 | 31.224 | 34.297 | 51.963 | 1.00 | 46.45 | 6 |
| 40 | ATOM | 972 | CG2 | ILE A | 392 | 31.241 | 34.582 | 50.479 | 1.00 | 42.35 | 6 |
| | ATOM | 973 | CG1 | ILE A | 392 | 29.791 | 33.953 | 52.402 | 1.00 | 49.69 | 6 |
| | ATOM | 974 | CD1 | ILE A | 392 | 28.792 | 35.039 | 52.113 | 1.00 | 51.09 | 6 |
| | ATOM | 975 | C | ILE A | 392 | 33.554 | 33.356 | 51.641 | 1.00 | 50.90 | 6 |
| | ATOM | 976 | O | ILE A | 392 | 33.914 | 32.605 | 50.732 | 1.00 | 52.21 | 8 |
| 45 | ATOM | 977 | N | GLU A | 393 | 34.298 | 34.374 | 52.071 | 1.00 | 50.43 | 7 |
| | ATOM | 978 | CA | GLU A | 393 | 35.592 | 34.684 | 51.471 | 1.00 | 50.30 | 6 |
| | ATOM | 979 | CB | GLU A | 393 | 36.437 | 35.561 | 52.387 | 1.00 | 53.97 | 6 |
| | ATOM | 980 | CG | GLU A | 393 | 36.558 | 36.966 | 51.844 | 1.00 | 62.18 | 6 |
| | ATOM | 981 | CD | GLU A | 393 | 37.546 | 37.777 | 52.564 | 1.00 | 67.69 | 6 |
| 50 | ATOM | 982 | OE1 | GLU A | 393 | 38.149 | 38.741 | 52.119 | 1.00 | 66.42 | 8 |
| | ATOM | 983 | OE2 | GLU A | 393 | 37.856 | 37.640 | 53.729 | 1.00 | 70.64 | 8 |
| | ATOM | 984 | C | GLU A | 393 | 36.341 | 33.429 | 51.230 | 1.00 | 49.31 | 6 |
| | ATOM | 985 | O | GLU A | 393 | 36.755 | 33.089 | 50.125 | 1.00 | 49.53 | 8 |
| | ATOM | 986 | N | LYS A | 394 | 36.552 | 32.730 | 52.303 | 1.00 | 46.07 | 7 |
| 55 | ATOM | 987 | CA | LYS A | 394 | 37.265 | 31.543 | 52.078 | 1.00 | 45.76 | 6 |
| | ATOM | 988 | CB | LYS A | 394 | 37.396 | 30.800 | 53.373 | 1.00 | 43.85 | 6 |
| | ATOM | 989 | CG | LYS A | 394 | 38.207 | 31.617 | 54.394 | 1.00 | 40.00 | 6 |
| | ATOM | 990 | CD | LYS A | 394 | 39.372 | 32.374 | 53.705 | 1.00 | 40.00 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 991 | CE | LYS | A | 394 | 40.136 | 33.205 | 54.681 | 1.00 | 40.00 | 6 |
| | ATOM | 992 | NZ | LYS | A | 394 | 41.516 | 33.602 | 54.162 | 1.00 | 40.00 | 7 |
| | ATOM | 993 | C | LYS | A | 394 | 36.568 | 30.778 | 50.966 | 1.00 | 46.69 | 6 |
| | ATOM | 994 | O | LYS | A | 394 | 37.215 | 30.427 | 49.988 | 1.00 | 49.13 | 8 |
| | ATOM | 995 | N | TYR | A | 395 | 35.269 | 30.514 | 51.095 | 1.00 | 46.57 | 7 |
| 10 | ATOM | 996 | CA | TYR | A | 395 | 34.553 | 29.823 | 50.022 | 1.00 | 43.33 | 6 |
| | ATOM | 997 | CB | TYR | A | 395 | 33.059 | 30.123 | 50.076 | 1.00 | 48.44 | 6 |
| | ATOM | 998 | CG | TYR | A | 395 | 32.275 | 29.236 | 50.994 | 1.00 | 53.83 | 6 |
| | ATOM | 999 | CD1 | TYR | A | 395 | 31.010 | 29.598 | 51.415 | 1.00 | 56.43 | 6 |
| | ATOM | 1000 | CE1 | TYR | A | 395 | 30.266 | 28.769 | 52.252 | 1.00 | 59.73 | 6 |
| 15 | ATOM | 1001 | CD2 | TYR | A | 395 | 32.790 | 28.033 | 51.428 | 1.00 | 56.47 | 6 |
| | ATOM | 1002 | CE2 | TYR | A | 395 | 32.054 | 27.198 | 52.265 | 1.00 | 62.60 | 6 |
| | ATOM | 1003 | CZ | TYR | A | 395 | 30.787 | 27.565 | 52.687 | 1.00 | 63.18 | 6 |
| | ATOM | 1004 | OH | TYR | A | 395 | 30.059 | 26.753 | 53.528 | 1.00 | 64.46 | 8 |
| | ATOM | 1005 | C | TYR | A | 395 | 35.120 | 30.356 | 48.716 | 1.00 | 37.30 | 6 |
| 20 | ATOM | 1006 | O | TYR | A | 395 | 35.643 | 29.601 | 47.908 | 1.00 | 34.10 | 8 |
| | ATOM | 1007 | N | GLN | A | 396 | 35.029 | 31.670 | 48.522 | 1.00 | 31.92 | 7 |
| | ATOM | 1008 | CA | GLN | A | 396 | 35.563 | 32.273 | 47.305 | 1.00 | 34.81 | 6 |
| | ATOM | 1009 | CB | GLN | A | 396 | 35.403 | 33.801 | 47.329 | 1.00 | 32.64 | 6 |
| | ATOM | 1010 | CG | GLN | A | 396 | 36.088 | 34.485 | 46.162 | 1.00 | 29.57 | 6 |
| 25 | ATOM | 1011 | CD | GLN | A | 396 | 35.616 | 35.891 | 45.927 | 1.00 | 29.46 | 6 |
| | ATOM | 1012 | OE1 | GLN | A | 396 | 35.599 | 36.726 | 46.862 | 1.00 | 34.65 | 8 |
| | ATOM | 1013 | NE2 | GLN | A | 396 | 35.245 | 36.173 | 44.689 | 1.00 | 27.21 | 7 |
| | ATOM | 1014 | C | GLN | A | 396 | 37.035 | 31.909 | 47.167 | 1.00 | 37.13 | 6 |
| | ATOM | 1015 | O | GLN | A | 396 | 37.511 | 31.590 | 46.080 | 1.00 | 37.36 | 8 |
| 30 | ATOM | 1016 | N | ASP | A | 397 | 37.751 | 31.970 | 48.285 | 1.00 | 38.61 | 7 |
| | ATOM | 1017 | CA | ASP | A | 397 | 39.164 | 31.642 | 48.298 | 1.00 | 40.37 | 6 |
| | ATOM | 1018 | CB | ASP | A | 397 | 39.757 | 31.869 | 49.704 | 1.00 | 40.51 | 6 |
| | ATOM | 1019 | CG | ASP | A | 397 | 39.813 | 33.319 | 50.095 | 1.00 | 43.77 | 6 |
| | ATOM | 1020 | OD1 | ASP | A | 397 | 40.397 | 34.123 | 49.334 | 1.00 | 46.50 | 8 |
| 35 | ATOM | 1021 | OD2 | ASP | A | 397 | 39.299 | 33.702 | 51.184 | 1.00 | 51.34 | 8 |
| | ATOM | 1022 | C | ASP | A | 397 | 39.302 | 30.176 | 47.898 | 1.00 | 38.62 | 6 |
| | ATOM | 1023 | O | ASP | A | 397 | 40.230 | 29.809 | 47.199 | 1.00 | 39.20 | 8 |
| | ATOM | 1024 | N | SER | A | 398 | 38.350 | 29.359 | 48.344 | 1.00 | 37.84 | 7 |
| | ATOM | 1025 | CA | SER | A | 398 | 38.348 | 27.929 | 48.063 | 1.00 | 37.80 | 6 |
| 40 | ATOM | 1026 | CB | SER | A | 398 | 37.240 | 27.240 | 48.878 | 1.00 | 34.28 | 6 |
| | ATOM | 1027 | OG | SER | A | 398 | 37.297 | 25.826 | 48.755 | 1.00 | 46.60 | 8 |
| | ATOM | 1028 | C | SER | A | 398 | 38.164 | 27.639 | 46.581 | 1.00 | 38.41 | 6 |
| | ATOM | 1029 | O | SER | A | 398 | 38.677 | 26.642 | 46.075 | 1.00 | 39.98 | 8 |
| | ATOM | 1030 | N | PHE | A | 399 | 37.419 | 28.507 | 45.893 | 1.00 | 34.82 | 7 |
| 45 | ATOM | 1031 | CA | PHE | A | 399 | 37.181 | 28.325 | 44.462 | 1.00 | 35.96 | 6 |
| | ATOM | 1032 | CB | PHE | A | 399 | 35.873 | 28.983 | 44.015 | 1.00 | 35.75 | 6 |
| | ATOM | 1033 | CG | PHE | A | 399 | 34.632 | 28.216 | 44.403 | 1.00 | 39.30 | 6 |
| | ATOM | 1034 | CD1 | PHE | A | 399 | 34.107 | 28.294 | 45.677 | 1.00 | 39.86 | 6 |
| | ATOM | 1035 | CD2 | PHE | A | 399 | 34.018 | 27.393 | 43.488 | 1.00 | 36.81 | 6 |
| 50 | ATOM | 1036 | CE1 | PHE | A | 399 | 32.961 | 27.557 | 46.013 | 1.00 | 41.25 | 6 |
| | ATOM | 1037 | CE2 | PHE | A | 399 | 32.880 | 26.661 | 43.825 | 1.00 | 43.61 | 6 |
| | ATOM | 1038 | CZ | PHE | A | 399 | 32.354 | 26.740 | 45.087 | 1.00 | 40.34 | 6 |
| | ATOM | 1039 | C | PHE | A | 399 | 38.328 | 28.890 | 43.630 | 1.00 | 33.48 | 6 |
| | ATOM | 1040 | O | PHE | A | 399 | 38.867 | 28.200 | 42.756 | 1.00 | 26.86 | 8 |
| 55 | ATOM | 1041 | N | LEU | A | 400 | 38.680 | 30.156 | 43.877 | 1.00 | 31.47 | 7 |
| | ATOM | 1042 | CA | LEU | A | 400 | 39.754 | 30.796 | 43.132 | 1.00 | 37.41 | 6 |
| | ATOM | 1043 | CB | LEU | A | 400 | 40.179 | 32.100 | 43.814 | 1.00 | 34.24 | 6 |
| | ATOM | 1044 | CG | LEU | A | 400 | 39.239 | 33.265 | 43.628 | 1.00 | 35.10 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 1045 | CD1 | LEU | A | 400 | 39.803 | 34.531 | 44.256 | 1.00 | 26.60 | 6 |
| | ATOM | 1046 | CD2 | LEU | A | 400 | 39.065 | 33.479 | 42.137 | 1.00 | 29.44 | 6 |
| | ATOM | 1047 | C | LEU | A | 400 | 40.941 | 29.872 | 42.947 | 1.00 | 38.84 | 6 |
| | ATOM | 1048 | O | LEU | A | 400 | 41.367 | 29.632 | 41.821 | 1.00 | 40.38 | 8 |
| | ATOM | 1049 | N | LEU | A | 401 | 41.464 | 29.350 | 44.055 | 1.00 | 42.79 | 7 |
| 10 | ATOM | 1050 | CA | LEU | A | 401 | 42.605 | 28.449 | 43.988 | 1.00 | 43.48 | 6 |
| | ATOM | 1051 | CB | LEU | A | 401 | 42.900 | 27.821 | 45.355 | 1.00 | 44.73 | 6 |
| | ATOM | 1052 | CG | LEU | A | 401 | 44.105 | 26.899 | 45.354 | 1.00 | 51.39 | 6 |
| | ATOM | 1053 | CD1 | LEU | A | 401 | 45.374 | 27.749 | 45.143 | 1.00 | 50.11 | 6 |
| | ATOM | 1054 | CD2 | LEU | A | 401 | 44.205 | 26.122 | 46.662 | 1.00 | 49.30 | 6 |
| 15 | ATOM | 1055 | C | LEU | A | 401 | 42.324 | 27.340 | 42.981 | 1.00 | 41.62 | 6 |
| | ATOM | 1056 | O | LEU | A | 401 | 43.052 | 27.180 | 42.004 | 1.00 | 45.14 | 8 |
| | ATOM | 1057 | N | ALA | A | 402 | 41.269 | 26.574 | 43.245 | 1.00 | 37.92 | 7 |
| | ATOM | 1058 | CA | ALA | A | 402 | 40.873 | 25.469 | 42.386 | 1.00 | 29.90 | 6 |
| | ATOM | 1059 | CB | ALA | A | 402 | 39.522 | 24.928 | 42.834 | 1.00 | 30.70 | 6 |
| 20 | ATOM | 1060 | C | ALA | A | 402 | 40.798 | 25.909 | 40.929 | 1.00 | 28.88 | 6 |
| | ATOM | 1061 | O | ALA | A | 402 | 41.277 | 25.203 | 40.034 | 1.00 | 32.14 | 8 |
| | ATOM | 1062 | N | PHE | A | 403 | 40.200 | 27.086 | 40.707 | 1.00 | 31.07 | 7 |
| | ATOM | 1063 | CA | PHE | A | 403 | 40.052 | 27.642 | 39.363 | 1.00 | 29.90 | 6 |
| | ATOM | 1064 | CB | PHE | A | 403 | 39.379 | 29.019 | 39.438 | 1.00 | 27.03 | 6 |
| 25 | ATOM | 1065 | CG | PHE | A | 403 | 38.943 | 29.574 | 38.100 | 1.00 | 26.97 | 6 |
| | ATOM | 1066 | CD1 | PHE | A | 403 | 38.228 | 30.758 | 38.033 | 1.00 | 25.55 | 6 |
| | ATOM | 1067 | CD2 | PHE | A | 403 | 39.224 | 28.905 | 36.925 | 1.00 | 19.75 | 6 |
| | ATOM | 1068 | CE1 | PHE | A | 403 | 37.784 | 31.266 | 36.808 | 1.00 | 27.90 | 6 |
| | ATOM | 1069 | CE2 | PHE | A | 403 | 38.780 | 29.416 | 35.694 | 1.00 | 22.56 | 6 |
| 30 | ATOM | 1070 | CZ | PHE | A | 403 | 38.063 | 30.596 | 35.640 | 1.00 | 22.24 | 6 |
| | ATOM | 1071 | C | PHE | A | 403 | 41.429 | 27.756 | 38.719 | 1.00 | 28.82 | 6 |
| | ATOM | 1072 | O | PHE | A | 403 | 41.666 | 27.210 | 37.646 | 1.00 | 26.00 | 8 |
| | ATOM | 1073 | N | GLU | A | 404 | 42.329 | 28.463 | 39.402 | 1.00 | 30.25 | 7 |
| | ATOM | 1074 | CA | GLU | A | 404 | 43.695 | 28.665 | 38.922 | 1.00 | 34.03 | 6 |
| 35 | ATOM | 1075 | CB | GLU | A | 404 | 44.513 | 29.416 | 39.983 | 1.00 | 39.45 | 6 |
| | ATOM | 1076 | CG | GLU | A | 404 | 45.867 | 29.935 | 39.489 | 1.00 | 47.68 | 6 |
| | ATOM | 1077 | CD | GLU | A | 404 | 46.734 | 30.507 | 40.571 | 1.00 | 54.02 | 6 |
| | ATOM | 1078 | OE1 | GLU | A | 404 | 46.236 | 31.298 | 41.408 | 1.00 | 57.27 | 8 |
| | ATOM | 1079 | OE2 | GLU | A | 404 | 47.956 | 30.202 | 40.606 | 1.00 | 63.85 | 8 |
| 40 | ATOM | 1080 | C | GLU | A | 404 | 44.352 | 27.322 | 38.634 | 1.00 | 36.01 | 6 |
| | ATOM | 1081 | O | GLU | A | 404 | 44.936 | 27.112 | 37.574 | 1.00 | 38.64 | 8 |
| | ATOM | 1082 | N | HIS | A | 405 | 44.259 | 26.420 | 39.610 | 1.00 | 29.56 | 7 |
| | ATOM | 1083 | CA | HIS | A | 405 | 44.840 | 25.093 | 39.468 | 1.00 | 31.69 | 6 |
| | ATOM | 1084 | CB | HIS | A | 405 | 44.540 | 24.228 | 40.694 | 1.00 | 33.75 | 6 |
| 45 | ATOM | 1085 | CG | HIS | A | 405 | 45.292 | 24.657 | 41.908 | 1.00 | 34.75 | 6 |
| | ATOM | 1086 | CD2 | HIS | A | 405 | 46.198 | 25.640 | 42.130 | 1.00 | 34.58 | 6 |
| | ATOM | 1087 | ND1 | HIS | A | 405 | 45.161 | 23.984 | 43.130 | 1.00 | 32.43 | 7 |
| | ATOM | 1088 | CE1 | HIS | A | 405 | 45.975 | 24.568 | 44.018 | 1.00 | 36.15 | 6 |
| | ATOM | 1089 | NE2 | HIS | A | 405 | 46.601 | 25.561 | 43.430 | 1.00 | 39.84 | 7 |
| 50 | ATOM | 1090 | C | HIS | A | 405 | 44.274 | 24.445 | 38.225 | 1.00 | 34.21 | 6 |
| | ATOM | 1091 | O | HIS | A | 405 | 45.029 | 23.949 | 37.386 | 1.00 | 37.06 | 8 |
| | ATOM | 1092 | N | TYR | A | 406 | 42.947 | 24.453 | 38.100 | 1.00 | 30.83 | 7 |
| | ATOM | 1093 | CA | TYR | A | 406 | 42.313 | 23.859 | 36.930 | 1.00 | 28.85 | 6 |
| | ATOM | 1094 | CB | TYR | A | 406 | 40.805 | 24.080 | 36.934 | 1.00 | 31.48 | 6 |
| 55 | ATOM | 1095 | CG | TYR | A | 406 | 40.139 | 23.494 | 35.709 | 1.00 | 23.49 | 6 |
| | ATOM | 1096 | CD1 | TYR | A | 406 | 40.073 | 22.123 | 35.532 | 1.00 | 19.42 | 6 |
| | ATOM | 1097 | CE1 | TYR | A | 406 | 39.517 | 21.577 | 34.382 | 1.00 | 23.80 | 6 |
| | ATOM | 1098 | CD2 | TYR | A | 406 | 39.646 | 24.313 | 34.704 | 1.00 | 21.81 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 1099 | CE2 | TYR | A | 406 | 39.090 | 23.351 | 33.380 | 1.00 | 21.56 | 6 |
| | ATOM | 1100 | CZ | TYR | A | 406 | 39.029 | 22.395 | 33.380 | 1.00 | 21.56 | 6 |
| | ATOM | 1101 | OH | TYR | A | 406 | 38.489 | 21.850 | 32.236 | 1.00 | 24.96 | 8 |
| | ATOM | 1102 | C | TYR | A | 406 | 42.882 | 24.504 | 35.672 | 1.00 | 24.24 | 6 |
| | ATOM | 1103 | O | TYR | A | 406 | 42.958 | 23.872 | 34.621 | 1.00 | 27.08 | 8 |
| 10 | ATOM | 1104 | N | ILE | A | 407 | 43.253 | 25.784 | 35.807 | 1.00 | 25.76 | 7 |
| | ATOM | 1105 | CA | ILE | A | 407 | 43.824 | 26.548 | 34.705 | 1.00 | 33.75 | 6 |
| | ATOM | 1106 | CB | ILE | A | 407 | 43.986 | 28.033 | 35.070 | 1.00 | 34.23 | 6 |
| | ATOM | 1107 | CG2 | ILE | A | 407 | 44.967 | 28.712 | 34.139 | 1.00 | 32.46 | 6 |
| | ATOM | 1108 | CG1 | ILE | A | 407 | 42.615 | 28.728 | 35.042 | 1.00 | 43.30 | 6 |
| 15 | ATOM | 1109 | CD1 | ILE | A | 407 | 41.896 | 28.602 | 33.694 | 1.00 | 40.40 | 6 |
| | ATOM | 1110 | C | ILE | A | 407 | 45.143 | 25.973 | 34.256 | 1.00 | 39.03 | 6 |
| | ATOM | 1111 | O | ILE | A | 407 | 45.383 | 25.771 | 33.063 | 1.00 | 35.18 | 8 |
| | ATOM | 1112 | N | ASN | A | 408 | 46.003 | 25.721 | 35.227 | 1.00 | 37.25 | 7 |
| | ATOM | 1113 | CA | ASN | A | 408 | 47.307 | 25.194 | 34.926 | 1.00 | 37.01 | 6 |
| 20 | ATOM | 1114 | CB | ASN | A | 408 | 48.107 | 25.017 | 36.213 | 1.00 | 32.27 | 6 |
| | ATOM | 1115 | CG | ASN | A | 408 | 48.346 | 26.362 | 36.936 | 1.00 | 33.56 | 6 |
| | ATOM | 1116 | OD1 | ASN | A | 408 | 48.827 | 27.335 | 36.320 | 1.00 | 31.99 | 8 |
| | ATOM | 1117 | ND2 | ASN | A | 408 | 48.038 | 26.403 | 38.231 | 1.00 | 31.23 | 7 |
| | ATOM | 1118 | C | ASN | A | 408 | 47.205 | 23.892 | 34.136 | 1.00 | 38.14 | 6 |
| 25 | ATOM | 1119 | O | ASN | A | 408 | 47.900 | 23.734 | 33.124 | 1.00 | 42.16 | 8 |
| | ATOM | 1120 | N | TYR | A | 409 | 46.334 | 22.981 | 34.568 | 1.00 | 35.62 | 7 |
| | ATOM | 1121 | CA | TYR | A | 409 | 46.159 | 21.710 | 33.866 | 1.00 | 35.91 | 6 |
| | ATOM | 1122 | CB | TYR | A | 409 | 45.051 | 20.859 | 34.507 | 1.00 | 34.41 | 6 |
| | ATOM | 1123 | CG | TYR | A | 409 | 44.624 | 19.687 | 33.619 | 1.00 | 38.73 | 6 |
| 30 | ATOM | 1124 | CD1 | TYR | A | 409 | 45.563 | 18.765 | 33.155 | 1.00 | 41.34 | 6 |
| | ATOM | 1125 | CE1 | TYR | A | 409 | 45.186 | 17.709 | 32.321 | 1.00 | 47.16 | 6 |
| | ATOM | 1126 | CD2 | TYR | A | 409 | 43.292 | 19.515 | 33.232 | 1.00 | 46.20 | 6 |
| | ATOM | 1127 | CE2 | TYR | A | 409 | 42.913 | 18.455 | 32.397 | 1.00 | 50.74 | 6 |
| | ATOM | 1128 | CZ | TYR | A | 409 | 43.863 | 17.551 | 31.946 | 1.00 | 50.88 | 6 |
| 35 | ATOM | 1129 | OH | TYR | A | 409 | 43.498 | 16.514 | 31.130 | 1.00 | 53.14 | 8 |
| | ATOM | 1130 | C | TYR | A | 409 | 45.760 | 21.966 | 32.424 | 1.00 | 38.16 | 6 |
| | ATOM | 1131 | O | TYR | A | 409 | 46.202 | 21.281 | 31.502 | 1.00 | 41.83 | 8 |
| | ATOM | 1132 | N | ARG | A | 410 | 44.872 | 22.943 | 32.272 | 1.00 | 42.25 | 7 |
| | ATOM | 1133 | CA | ARG | A | 410 | 44.345 | 23.332 | 30.984 | 1.00 | 42.83 | 6 |
| 40 | ATOM | 1134 | CB | ARG | A | 410 | 43.311 | 24.427 | 31.195 | 1.00 | 36.83 | 6 |
| | ATOM | 1135 | CG | ARG | A | 410 | 41.994 | 23.979 | 31.795 | 1.00 | 34.32 | 6 |
| | ATOM | 1136 | CD | ARG | A | 410 | 41.073 | 23.504 | 30.675 | 1.00 | 36.62 | 6 |
| | ATOM | 1137 | NE | ARG | A | 410 | 40.888 | 24.550 | 29.685 | 1.00 | 38.64 | 7 |
| | ATOM | 1138 | CZ | ARG | A | 410 | 40.177 | 24.397 | 28.576 | 1.00 | 35.73 | 6 |
| 45 | ATOM | 1139 | NH1 | ARG | A | 410 | 39.572 | 23.230 | 28.348 | 1.00 | 33.17 | 7 |
| | ATOM | 1140 | NH2 | ARG | A | 410 | 40.077 | 25.407 | 27.708 | 1.00 | 32.70 | 7 |
| | ATOM | 1141 | C | ARG | A | 410 | 45.442 | 23.850 | 30.083 | 1.00 | 46.67 | 6 |
| | ATOM | 1142 | O | ARG | A | 410 | 45.467 | 23.591 | 28.882 | 1.00 | 41.78 | 8 |
| | ATOM | 1143 | N | LYS | A | 411 | 46.360 | 24.577 | 30.710 | 1.00 | 52.99 | 7 |
| 50 | ATOM | 1144 | CA | LYS | A | 411 | 47.467 | 25.194 | 30.017 | 1.00 | 58.32 | 6 |
| | ATOM | 1145 | CB | LYS | A | 411 | 48.645 | 24.216 | 29.876 | 1.00 | 64.99 | 6 |
| | ATOM | 1146 | CG | LYS | A | 411 | 48.349 | 22.835 | 29.367 | 1.00 | 70.48 | 6 |
| | ATOM | 1147 | CD | LYS | A | 411 | 49.608 | 21.974 | 29.494 | 1.00 | 77.18 | 6 |
| | ATOM | 1148 | CE | LYS | A | 411 | 49.461 | 20.621 | 28.795 | 1.00 | 84.30 | 6 |
| 55 | ATOM | 1149 | NZ | LYS | A | 411 | 50.740 | 19.828 | 28.857 | 1.00 | 86.48 | 7 |
| | ATOM | 1150 | C | LYS | A | 411 | 47.032 | 25.756 | 28.686 | 1.00 | 56.66 | 6 |
| | ATOM | 1151 | O | LYS | A | 411 | 47.160 | 25.153 | 27.633 | 1.00 | 55.47 | 8 |
| | ATOM | 1152 | N | HIS | A | 412 | 46.458 | 26.943 | 28.823 | 1.00 | 54.67 | 7 |

| | | | | | | | | | | | | |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 1153 | CA | HIS | A | 412 | 45.984 | 27.722 | 27.705 | 1.00 | 48.67 | 6 |
| | ATOM | 1154 | CB | HIS | A | 412 | 45.124 | 28.884 | 28.201 | 1.00 | 43.14 | 6 |
| | ATOM | 1155 | CG | HIS | A | 412 | 43.812 | 28.480 | 28.755 | 1.00 | 41.36 | 6 |
| | ATOM | 1156 | CD2 | HIS | A | 412 | 43.429 | 28.064 | 29.987 | 1.00 | 35.44 | 6 |
| | ATOM | 1157 | ND1 | HIS | A | 412 | 42.651 | 28.440 | 27.966 | 1.00 | 38.19 | 7 |
| 10 | ATOM | 1158 | CE1 | HIS | A | 412 | 41.648 | 28.014 | 28.723 | 1.00 | 34.75 | 6 |
| | ATOM | 1159 | NE2 | HIS | A | 412 | 42.094 | 27.780 | 29.942 | 1.00 | 35.52 | 7 |
| | ATOM | 1160 | C | HIS | A | 412 | 47.231 | 28.303 | 27.101 | 1.00 | 46.35 | 6 |
| | ATOM | 1161 | O | HIS | A | 412 | 48.269 | 28.452 | 27.775 | 1.00 | 42.73 | 8 |
| | ATOM | 1162 | N | HIS | A | 413 | 47.116 | 28.696 | 25.839 | 1.00 | 48.92 | 7 |
| 15 | ATOM | 1163 | CA | HIS | A | 413 | 48.234 | 29.290 | 25.146 | 1.00 | 53.15 | 6 |
| | ATOM | 1164 | CB | HIS | A | 413 | 48.404 | 28.666 | 23.755 | 1.00 | 55.27 | 6 |
| | ATOM | 1165 | CG | HIS | A | 413 | 49.326 | 29.446 | 22.886 | 1.00 | 58.77 | 6 |
| | ATOM | 1166 | CD2 | HIS | A | 413 | 49.213 | 30.660 | 22.304 | 1.00 | 61.65 | 6 |
| | ATOM | 1167 | ND1 | HIS | A | 413 | 50.617 | 28.997 | 22.564 | 1.00 | 60.31 | 7 |
| 20 | ATOM | 1168 | CE1 | HIS | A | 413 | 51.214 | 29.924 | 21.828 | 1.00 | 63.01 | 6 |
| | ATOM | 1169 | NE2 | HIS | A | 413 | 50.386 | 30.941 | 21.658 | 1.00 | 62.93 | 7 |
| | ATOM | 1170 | C | HIS | A | 413 | 47.932 | 30.768 | 24.998 | 1.00 | 53.19 | 6 |
| | ATOM | 1171 | O | HIS | A | 413 | 47.639 | 31.301 | 23.934 | 1.00 | 54.93 | 8 |
| | ATOM | 1172 | N | VAL | A | 414 | 47.964 | 31.413 | 26.139 | 1.00 | 53.77 | 7 |
| 25 | ATOM | 1173 | CA | VAL | A | 414 | 47.735 | 32.811 | 26.146 | 1.00 | 51.06 | 6 |
| | ATOM | 1174 | CB | VAL | A | 414 | 46.291 | 33.183 | 26.417 | 1.00 | 51.49 | 6 |
| | ATOM | 1175 | CG1 | VAL | A | 414 | 46.186 | 34.715 | 26.603 | 1.00 | 45.22 | 6 |
| | ATOM | 1176 | CG2 | VAL | A | 414 | 45.419 | 32.732 | 25.263 | 1.00 | 52.67 | 6 |
| | ATOM | 1177 | C | VAL | A | 414 | 48.623 | 33.283 | 27.226 | 1.00 | 54.28 | 6 |
| 30 | ATOM | 1178 | O | VAL | A | 414 | 48.427 | 33.029 | 28.409 | 1.00 | 55.49 | 8 |
| | ATOM | 1179 | N | THR | A | 415 | 49.706 | 33.863 | 26.733 | 1.00 | 56.28 | 7 |
| | ATOM | 1180 | CA | THR | A | 415 | 50.721 | 34.484 | 27.557 | 1.00 | 57.83 | 6 |
| | ATOM | 1181 | CB | THR | A | 415 | 51.268 | 35.675 | 26.758 | 1.00 | 59.64 | 6 |
| | ATOM | 1182 | OG1 | THR | A | 415 | 51.605 | 36.754 | 27.636 | 1.00 | 66.69 | 8 |
| 35 | ATOM | 1183 | CG2 | THR | A | 415 | 50.197 | 36.158 | 25.745 | 1.00 | 59.42 | 6 |
| | ATOM | 1184 | C | THR | A | 415 | 50.146 | 35.049 | 28.879 | 1.00 | 56.98 | 6 |
| | ATOM | 1185 | O | THR | A | 415 | 48.933 | 35.146 | 29.051 | 1.00 | 55.70 | 8 |
| | ATOM | 1186 | N | HIS | A | 416 | 51.068 | 35.330 | 29.795 | 1.00 | 57.44 | 7 |
| | ATOM | 1187 | CA | HIS | A | 416 | 50.808 | 36.011 | 31.047 | 1.00 | 57.34 | 6 |
| 40 | ATOM | 1188 | CB | HIS | A | 416 | 51.346 | 37.422 | 30.708 | 1.00 | 61.35 | 6 |
| | ATOM | 1189 | CG | HIS | A | 416 | 51.872 | 38.237 | 31.821 | 1.00 | 69.78 | 6 |
| | ATOM | 1190 | CD2 | HIS | A | 416 | 53.114 | 38.297 | 32.390 | 1.00 | 71.42 | 6 |
| | ATOM | 1191 | ND1 | HIS | A | 416 | 51.135 | 39.263 | 32.416 | 1.00 | 72.49 | 7 |
| | ATOM | 1192 | CE1 | HIS | A | 416 | 51.914 | 39.884 | 33.290 | 1.00 | 75.50 | 6 |
| 45 | ATOM | 1193 | NE2 | HIS | A | 416 | 53.099 | 39.323 | 33.291 | 1.00 | 73.91 | 7 |
| | ATOM | 1194 | C | HIS | A | 416 | 49.261 | 35.892 | 31.297 | 1.00 | 53.79 | 6 |
| | ATOM | 1195 | O | HIS | A | 416 | 48.499 | 36.779 | 30.902 | 1.00 | 52.81 | 8 |
| | ATOM | 1196 | N | PHE | A | 417 | 48.806 | 34.779 | 31.911 | 1.00 | 48.05 | 7 |
| | ATOM | 1197 | CA | PHE | A | 417 | 47.355 | 34.428 | 32.061 | 1.00 | 47.99 | 6 |
| 50 | ATOM | 1198 | CB | PHE | A | 417 | 47.165 | 32.954 | 31.996 | 1.00 | 46.11 | 6 |
| | ATOM | 1199 | CG | PHE | A | 417 | 45.835 | 32.590 | 31.399 | 1.00 | 44.27 | 6 |
| | ATOM | 1200 | CD1 | PHE | A | 417 | 45.680 | 32.720 | 30.046 | 1.00 | 41.79 | 6 |
| | ATOM | 1201 | CD2 | PHE | A | 417 | 44.758 | 32.135 | 32.164 | 1.00 | 40.23 | 6 |
| | ATOM | 1202 | CE1 | PHE | A | 417 | 44.498 | 32.397 | 29.422 | 1.00 | 44.30 | 6 |
| 55 | ATOM | 1203 | CE2 | PHE | A | 417 | 43.540 | 31.802 | 31.529 | 1.00 | 36.80 | 6 |
| | ATOM | 1204 | CZ | PHE | A | 417 | 43.427 | 31.928 | 30.144 | 1.00 | 40.69 | 6 |
| | ATOM | 1205 | C | PHE | A | 417 | 46.427 | 34.836 | 33.196 | 1.00 | 46.69 | 6 |
| | ATOM | 1206 | O | PHE | A | 417 | 46.147 | 36.004 | 33.331 | 1.00 | 43.35 | 8 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| 5 | ATOM | 1207 | N | TRP | A | 418 | 45.906 | 33.801 | 33.909 | 1.00 | 45.14 | 7 |
| | ATOM | 1208 | CA | TRP | A | 418 | 44.982 | 33.867 | 35.065 | 1.00 | 44.89 | 6 |
| | ATOM | 1209 | CB | TRP | A | 418 | 45.545 | 33.099 | 36.255 | 1.00 | 42.24 | 6 |
| | ATOM | 1210 | CG | TRP | A | 418 | 44.959 | 33.452 | 37.598 | 1.00 | 47.11 | 6 |
| | ATOM | 1211 | CD2 | TRP | A | 418 | 43.724 | 32.924 | 38.149 | 1.00 | 46.98 | 6 |
| 10 | ATOM | 1212 | CE2 | TRP | A | 418 | 43.534 | 33.565 | 39.413 | 1.00 | 48.94 | 6 |
| | ATOM | 1213 | CE3 | TRP | A | 418 | 42.777 | 31.986 | 37.688 | 1.00 | 45.23 | 6 |
| | ATOM | 1214 | CD1 | TRP | A | 418 | 45.434 | 34.350 | 38.512 | 1.00 | 46.24 | 6 |
| | ATOM | 1215 | NE1 | TRP | A | 418 | 44.588 | 34.407 | 39.608 | 1.00 | 50.63 | 7 |
| | ATOM | 1216 | CZ2 | TRP | A | 418 | 42.441 | 33.270 | 40.238 | 1.00 | 45.46 | 6 |
| 15 | ATOM | 1217 | CZ3 | TRP | A | 418 | 41.686 | 31.706 | 38.500 | 1.00 | 44.50 | 6 |
| | ATOM | 1218 | CH2 | TRP | A | 418 | 41.511 | 32.335 | 39.753 | 1.00 | 47.55 | 6 |
| | ATOM | 1219 | C | TRP | A | 418 | 44.908 | 35.324 | 35.398 | 1.00 | 43.88 | 6 |
| | ATOM | 1220 | O | TRP | A | 418 | 43.797 | 35.839 | 35.702 | 1.00 | 43.17 | 8 |
| | ATOM | 1221 | N | PRO | A | 419 | 46.084 | 35.976 | 35.461 | 1.00 | 43.55 | 7 |
| 20 | ATOM | 1222 | CD | PRO | A | 419 | 47.467 | 35.482 | 35.400 | 1.00 | 41.52 | 6 |
| | ATOM | 1223 | CA | PRO | A | 419 | 46.009 | 37.396 | 35.758 | 1.00 | 41.48 | 6 |
| | ATOM | 1224 | CB | PRO | A | 419 | 47.436 | 37.884 | 35.535 | 1.00 | 39.21 | 6 |
| | ATOM | 1225 | CG | PRO | A | 419 | 48.261 | 36.696 | 35.223 | 1.00 | 39.25 | 6 |
| | ATOM | 1226 | C | PRO | A | 419 | 44.960 | 38.090 | 34.817 | 1.00 | 36.28 | 6 |
| 25 | ATOM | 1227 | O | PRO | A | 419 | 44.208 | 38.978 | 35.237 | 1.00 | 37.08 | 8 |
| | ATOM | 1228 | N | LYS | A | 420 | 44.915 | 37.701 | 33.540 | 1.00 | 35.96 | 7 |
| | ATOM | 1229 | CA | LYS | A | 420 | 43.977 | 38.287 | 32.575 | 1.00 | 40.82 | 6 |
| | ATOM | 1230 | CB | LYS | A | 420 | 44.314 | 37.805 | 31.155 | 1.00 | 40.78 | 6 |
| | ATOM | 1231 | CG | LYS | A | 420 | 45.684 | 38.244 | 30.641 | 1.00 | 48.62 | 6 |
| 30 | ATOM | 1232 | CD | LYS | A | 420 | 45.904 | 37.781 | 29.206 | 1.00 | 55.12 | 6 |
| | ATOM | 1233 | CE | LYS | A | 420 | 47.248 | 38.261 | 28.673 | 1.00 | 53.26 | 6 |
| | ATOM | 1234 | NZ | LYS | A | 420 | 47.448 | 37.884 | 27.222 | 1.00 | 52.69 | 7 |
| | ATOM | 1235 | C | LYS | A | 420 | 42.580 | 37.832 | 32.948 | 1.00 | 40.29 | 6 |
| | ATOM | 1236 | O | LYS | A | 420 | 41.656 | 38.626 | 32.982 | 1.00 | 39.66 | 8 |
| 35 | ATOM | 1237 | N | LEU | A | 421 | 42.461 | 36.537 | 33.245 | 1.00 | 38.33 | 7 |
| | ATOM | 1238 | CA | LEU | A | 421 | 41.186 | 35.931 | 33.613 | 1.00 | 37.60 | 6 |
| | ATOM | 1239 | CB | LEU | A | 421 | 41.397 | 34.433 | 33.915 | 1.00 | 43.66 | 6 |
| | ATOM | 1240 | CG | LEU | A | 421 | 40.204 | 33.518 | 33.828 | 1.00 | 46.50 | 6 |
| | ATOM | 1241 | CD1 | LEU | A | 421 | 39.643 | 33.624 | 32.426 | 1.00 | 45.15 | 6 |
| 40 | ATOM | 1242 | CD2 | LEU | A | 421 | 40.595 | 32.094 | 34.131 | 1.00 | 51.31 | 6 |
| | ATOM | 1243 | C | LEU | A | 421 | 40.575 | 36.664 | 34.808 | 1.00 | 39.59 | 6 |
| | ATOM | 1244 | O | LEU | A | 421 | 39.371 | 36.910 | 34.837 | 1.00 | 40.66 | 8 |
| | ATOM | 1245 | N | LEU | A | 422 | 41.412 | 37.017 | 35.782 | 1.00 | 39.57 | 7 |
| | ATOM | 1246 | CA | LEU | A | 422 | 40.946 | 37.726 | 36.961 | 1.00 | 38.63 | 6 |
| 45 | ATOM | 1247 | CB | LEU | A | 422 | 42.085 | 37.890 | 37.971 | 1.00 | 41.79 | 6 |
| | ATOM | 1248 | CG | LEU | A | 422 | 42.424 | 36.671 | 38.798 | 1.00 | 42.74 | 6 |
| | ATOM | 1249 | CD1 | LEU | A | 422 | 43.490 | 37.010 | 39.820 | 1.00 | 42.89 | 6 |
| | ATOM | 1250 | CD2 | LEU | A | 422 | 41.168 | 36.216 | 39.523 | 1.00 | 39.27 | 6 |
| | ATOM | 1251 | C | LEU | A | 422 | 40.381 | 39.073 | 36.589 | 1.00 | 40.47 | 6 |
| 50 | ATOM | 1252 | O | LEU | A | 422 | 39.428 | 39.525 | 37.210 | 1.00 | 47.83 | 8 |
| | ATOM | 1253 | N | MET | A | 423 | 40.969 | 39.698 | 35.569 | 1.00 | 34.27 | 7 |
| | ATOM | 1254 | CA | MET | A | 423 | 40.511 | 41.001 | 35.117 | 1.00 | 35.25 | 6 |
| | ATOM | 1255 | CB | MET | A | 423 | 41.427 | 41.553 | 34.028 | 1.00 | 32.56 | 6 |
| | ATOM | 1256 | CG | MET | A | 423 | 42.856 | 41.732 | 34.456 | 1.00 | 40.70 | 6 |
| 55 | ATOM | 1257 | SD | MET | A | 423 | 43.707 | 43.101 | 33.619 | 1.00 | 47.65 | 16 |
| | ATOM | 1258 | CE | MET | A | 423 | 43.348 | 42.776 | 31.848 | 1.00 | 47.16 | 6 |
| | ATOM | 1259 | C | MET | A | 423 | 39.100 | 40.899 | 34.574 | 1.00 | 35.13 | 6 |
| | ATOM | 1260 | O | MET | A | 423 | 38.315 | 41.829 | 34.696 | 1.00 | 29.85 | 8 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 1261 | N | LYS | A | 424 | 38.791 | 39.752 | 33.975 | 1.00 | 31.56 | 7 |
| | ATOM | 1262 | CA | LYS | A | 424 | 37.470 | 39.529 | 33.423 | 1.00 | 32.29 | 6 |
| | ATOM | 1263 | CB | LYS | A | 424 | 37.446 | 38.205 | 32.658 | 1.00 | 30.56 | 6 |
| | ATOM | 1264 | CG | LYS | A | 424 | 38.394 | 38.192 | 31.455 | 1.00 | 30.07 | 6 |
| | ATOM | 1265 | CD | LYS | A | 424 | 38.050 | 39.326 | 30.488 | 1.00 | 33.22 | 6 |
| 10 | ATOM | 1266 | CE | LYS | A | 424 | 39.032 | 39.433 | 29.322 | 1.00 | 28.75 | 6 |
| | ATOM | 1267 | NZ | LYS | A | 424 | 40.394 | 39.942 | 29.707 | 1.00 | 31.01 | 7 |
| | ATOM | 1268 | C | LYS | A | 424 | 36.418 | 39.558 | 34.524 | 1.00 | 29.26 | 6 |
| | ATOM | 1269 | O | LYS | A | 424 | 35.307 | 39.998 | 34.289 | 1.00 | 30.22 | 8 |
| | ATOM | 1270 | N | VAL | A | 425 | 36.796 | 39.098 | 35.719 | 1.00 | 23.53 | 7 |
| 15 | ATOM | 1271 | CA | VAL | A | 425 | 35.897 | 39.107 | 36.866 | 1.00 | 28.91 | 6 |
| | ATOM | 1272 | CB | VAL | A | 425 | 36.541 | 38.460 | 38.094 | 1.00 | 29.44 | 6 |
| | ATOM | 1273 | CG1 | VAL | A | 425 | 35.673 | 38.642 | 39.320 | 1.00 | 28.81 | 6 |
| | ATOM | 1274 | CG2 | VAL | A | 425 | 36.764 | 36.985 | 37.849 | 1.00 | 31.22 | 6 |
| | ATOM | 1275 | C | VAL | A | 425 | 35.512 | 40.548 | 37.161 | 1.00 | 32.03 | 6 |
| 20 | ATOM | 1276 | O | VAL | A | 425 | 34.350 | 40.839 | 37.429 | 1.00 | 31.95 | 8 |
| | ATOM | 1277 | N | THR | A | 426 | 36.496 | 41.444 | 37.124 | 1.00 | 33.61 | 7 |
| | ATOM | 1278 | CA | THR | A | 426 | 36.248 | 42.866 | 37.356 | 1.00 | 30.76 | 6 |
| | ATOM | 1279 | CB | THR | A | 426 | 37.559 | 43.670 | 37.360 | 1.00 | 32.34 | 6 |
| | ATOM | 1280 | OG1 | THR | A | 426 | 38.209 | 43.565 | 38.630 | 1.00 | 33.07 | 8 |
| 25 | ATOM | 1281 | CG2 | THR | A | 426 | 37.302 | 45.131 | 37.015 | 1.00 | 25.40 | 6 |
| | ATOM | 1282 | C | THR | A | 426 | 35.363 | 43.324 | 36.211 | 1.00 | 32.53 | 6 |
| | ATOM | 1283 | O | THR | A | 426 | 34.357 | 44.006 | 36.405 | 1.00 | 35.19 | 8 |
| | ATOM | 1284 | N | ASP | A | 427 | 35.763 | 42.929 | 35.006 | 1.00 | 28.83 | 7 |
| | ATOM | 1285 | CA | ASP | A | 427 | 35.011 | 43.272 | 33.810 | 1.00 | 35.12 | 6 |
| 30 | ATOM | 1286 | CB | ASP | A | 427 | 35.556 | 42.524 | 32.578 | 1.00 | 39.14 | 6 |
| | ATOM | 1287 | CG | ASP | A | 427 | 36.837 | 43.103 | 32.057 | 1.00 | 45.80 | 6 |
| | ATOM | 1288 | OD1 | ASP | A | 427 | 36.982 | 44.346 | 32.024 | 1.00 | 41.97 | 8 |
| | ATOM | 1289 | OD2 | ASP | A | 427 | 37.735 | 42.333 | 31.616 | 1.00 | 50.06 | 8 |
| | ATOM | 1290 | C | ASP | A | 427 | 33.537 | 42.925 | 34.028 | 1.00 | 33.94 | 6 |
| 35 | ATOM | 1291 | O | ASP | A | 427 | 32.659 | 43.712 | 33.702 | 1.00 | 38.02 | 8 |
| | ATOM | 1292 | N | LEU | A | 428 | 33.283 | 41.745 | 34.584 | 1.00 | 27.15 | 7 |
| | ATOM | 1293 | CA | LEU | A | 428 | 31.925 | 41.293 | 34.850 | 1.00 | 29.99 | 6 |
| | ATOM | 1294 | CB | LEU | A | 428 | 31.924 | 39.786 | 35.133 | 1.00 | 22.49 | 6 |
| | ATOM | 1295 | CG | LEU | A | 428 | 32.104 | 38.873 | 33.939 | 1.00 | 25.54 | 6 |
| 40 | ATOM | 1296 | CD1 | LEU | A | 428 | 32.202 | 37.421 | 34.353 | 1.00 | 20.60 | 6 |
| | ATOM | 1297 | CD2 | LEU | A | 428 | 30.920 | 39.083 | 33.029 | 1.00 | 17.24 | 6 |
| | ATOM | 1298 | C | LEU | A | 428 | 31.276 | 42.057 | 35.991 | 1.00 | 28.94 | 6 |
| | ATOM | 1299 | O | LEU | A | 428 | 30.082 | 42.306 | 35.939 | 1.00 | 31.26 | 8 |
| | ATOM | 1300 | N | ARG | A | 429 | 32.059 | 42.423 | 37.011 | 1.00 | 27.64 | 7 |
| 45 | ATOM | 1301 | CA | ARG | A | 429 | 31.527 | 43.162 | 38.147 | 1.00 | 28.13 | 6 |
| | ATOM | 1302 | CB | ARG | A | 429 | 32.564 | 43.298 | 39.264 | 1.00 | 29.59 | 6 |
| | ATOM | 1303 | CG | ARG | A | 429 | 32.818 | 42.040 | 40.080 | 1.00 | 34.85 | 6 |
| | ATOM | 1304 | CD | ARG | A | 429 | 33.588 | 42.360 | 41.367 | 1.00 | 47.18 | 6 |
| | ATOM | 1305 | NE | ARG | A | 429 | 34.093 | 41.175 | 42.049 | 1.00 | 57.93 | 7 |
| 50 | ATOM | 1306 | CZ | ARG | A | 429 | 33.327 | 40.210 | 42.547 | 1.00 | 63.62 | 6 |
| | ATOM | 1307 | NH1 | ARG | A | 429 | 31.998 | 40.270 | 42.396 | 1.00 | 60.71 | 7 |
| | ATOM | 1308 | NH2 | ARG | A | 429 | 33.900 | 39.165 | 43.150 | 1.00 | 62.38 | 7 |
| | ATOM | 1309 | C | ARG | A | 429 | 31.099 | 44.536 | 37.707 | 1.00 | 29.81 | 6 |
| | ATOM | 1310 | O | ARG | A | 429 | 30.044 | 45.009 | 38.101 | 1.00 | 30.81 | 8 |
| 55 | ATOM | 1311 | N | MET | A | 430 | 31.941 | 45.176 | 36.901 | 1.00 | 29.64 | 7 |
| | ATOM | 1312 | CA | MET | A | 430 | 31.644 | 46.502 | 36.383 | 1.00 | 34.72 | 6 |
| | ATOM | 1313 | CB | MET | A | 430 | 32.745 | 46.955 | 35.434 | 1.00 | 34.97 | 6 |
| | ATOM | 1314 | CG | MET | A | 430 | 33.937 | 47.597 | 36.080 | 1.00 | 45.34 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| 5 | ATOM | 1315 | SD | MET | A | 430 | 33.520 | 49.120 | 36.937 | 1.00 | 52.55 | 16 |
| | ATOM | 1316 | CE | MET | A | 430 | 32.942 | 50.174 | 35.585 | 1.00 | 55.56 | 6 |
| | ATOM | 1317 | C | MET | A | 430 | 30.315 | 46.455 | 35.634 | 1.00 | 34.01 | 6 |
| | ATOM | 1318 | O | MET | A | 430 | 29.455 | 47.295 | 35.854 | 1.00 | 37.29 | 8 |
| | ATOM | 1319 | N | ILE | A | 431 | 30.180 | 45.468 | 34.740 | 1.00 | 29.99 | 7 |
| 10 | ATOM | 1320 | CA | ILE | A | 431 | 28.954 | 45.269 | 33.969 | 1.00 | 28.82 | 6 |
| | ATOM | 1321 | CB | ILE | A | 431 | 28.962 | 43.936 | 33.211 | 1.00 | 27.39 | 6 |
| | ATOM | 1322 | CG2 | ILE | A | 431 | 27.622 | 43.671 | 32.572 | 1.00 | 23.87 | 6 |
| | ATOM | 1323 | CG1 | ILE | A | 431 | 30.044 | 43.920 | 32.138 | 1.00 | 25.56 | 6 |
| | ATOM | 1324 | CD1 | ILE | A | 431 | 29.989 | 42.703 | 31.244 | 1.00 | 17.29 | 6 |
| 15 | ATOM | 1325 | C | ILE | A | 431 | 27.769 | 45.269 | 34.907 | 1.00 | 29.49 | 6 |
| | ATOM | 1326 | O | ILE | A | 431 | 26.810 | 45.993 | 34.712 | 1.00 | 24.19 | 8 |
| | ATOM | 1327 | N | GLY | A | 432 | 27.839 | 44.435 | 35.936 | 1.00 | 25.25 | 7 |
| | ATOM | 1328 | CA | GLY | A | 432 | 26.748 | 44.343 | 36.890 | 1.00 | 30.38 | 6 |
| | ATOM | 1329 | C | GLY | A | 432 | 26.494 | 45.671 | 37.554 | 1.00 | 32.75 | 6 |
| 20 | ATOM | 1330 | O | GLY | A | 432 | 25.411 | 46.206 | 37.469 | 1.00 | 36.38 | 8 |
| | ATOM | 1331 | N | ALA | A | 433 | 27.514 | 46.189 | 38.221 | 1.00 | 26.77 | 7 |
| | ATOM | 1332 | CA | ALA | A | 433 | 27.428 | 47.459 | 38.910 | 1.00 | 26.48 | 6 |
| | ATOM | 1333 | CB | ALA | A | 433 | 28.836 | 47.970 | 39.203 | 1.00 | 19.90 | 6 |
| | ATOM | 1334 | C | ALA | A | 433 | 26.663 | 48.502 | 38.114 | 1.00 | 30.73 | 6 |
| 25 | ATOM | 1335 | O | ALA | A | 433 | 25.773 | 49.164 | 38.635 | 1.00 | 31.60 | 8 |
| | ATOM | 1336 | N | CYS | A | 434 | 27.027 | 48.654 | 36.854 | 1.00 | 33.22 | 7 |
| | ATOM | 1337 | CA | CYS | A | 434 | 26.371 | 49.616 | 35.996 | 1.00 | 34.34 | 6 |
| | ATOM | 1338 | CB | CYS | A | 434 | 27.047 | 49.612 | 34.711 | 1.00 | 35.20 | 6 |
| | ATOM | 1339 | SG | CYS | A | 434 | 27.789 | 50.811 | 34.285 | 1.00 | 54.48 | 16 |
| 30 | ATOM | 1340 | C | CYS | A | 434 | 24.974 | 49.198 | 35.612 | 1.00 | 34.09 | 6 |
| | ATOM | 1341 | O | CYS | A | 434 | 24.107 | 50.040 | 35.415 | 1.00 | 34.89 | 8 |
| | ATOM | 1342 | N | HIS | A | 435 | 24.756 | 47.898 | 35.447 | 1.00 | 34.30 | 7 |
| | ATOM | 1343 | CA | HIS | A | 435 | 23.453 | 47.423 | 35.042 | 1.00 | 35.44 | 6 |
| | ATOM | 1344 | CB | HIS | A | 435 | 23.404 | 45.904 | 35.104 | 1.00 | 31.76 | 6 |
| 35 | ATOM | 1345 | CG | HIS | A | 435 | 22.099 | 45.351 | 34.675 | 1.00 | 32.03 | 6 |
| | ATOM | 1346 | CD2 | HIS | A | 435 | 21.697 | 44.790 | 33.519 | 1.00 | 28.61 | 6 |
| | ATOM | 1347 | ND1 | HIS | A | 435 | 20.941 | 45.482 | 35.452 | 1.00 | 28.48 | 7 |
| | ATOM | 1348 | CE1 | HIS | A | 435 | 19.912 | 45.025 | 34.759 | 1.00 | 33.27 | 6 |
| | ATOM | 1349 | NE2 | HIS | A | 435 | 20.345 | 44.597 | 33.583 | 1.00 | 31.57 | 7 |
| 40 | ATOM | 1350 | C | HIS | A | 435 | 22.400 | 47.974 | 35.972 | 1.00 | 32.74 | 6 |
| | ATOM | 1351 | O | HIS | A | 435 | 21.304 | 48.284 | 35.565 | 1.00 | 32.87 | 8 |
| | ATOM | 1352 | N | ALA | A | 436 | 22.777 | 48.046 | 37.241 | 1.00 | 31.01 | 7 |
| | ATOM | 1353 | CA | ALA | A | 436 | 21.910 | 48.563 | 38.266 | 1.00 | 29.91 | 6 |
| | ATOM | 1354 | CB | ALA | A | 436 | 22.661 | 48.595 | 39.580 | 1.00 | 21.23 | 6 |
| 45 | ATOM | 1355 | C | ALA | A | 436 | 21.475 | 49.969 | 37.884 | 1.00 | 33.86 | 6 |
| | ATOM | 1356 | O | ALA | A | 436 | 20.296 | 50.298 | 37.910 | 1.00 | 36.10 | 8 |
| | ATOM | 1357 | N | SER | A | 437 | 22.453 | 50.795 | 37.532 | 1.00 | 35.19 | 7 |
| | ATOM | 1358 | CA | SER | A | 437 | 22.172 | 52.167 | 37.140 | 1.00 | 33.03 | 6 |
| | ATOM | 1359 | CB | SER | A | 437 | 23.441 | 52.815 | 36.603 | 1.00 | 35.31 | 6 |
| 50 | ATOM | 1360 | OG | SER | A | 437 | 23.203 | 54.151 | 36.193 | 1.00 | 44.99 | 8 |
| | ATOM | 1361 | C | SER | A | 437 | 21.110 | 52.158 | 36.055 | 1.00 | 38.39 | 6 |
| | ATOM | 1362 | O | SER | A | 437 | 20.049 | 52.745 | 36.204 | 1.00 | 37.54 | 8 |
| | ATOM | 1363 | N | ARG | A | 438 | 21.432 | 51.483 | 34.956 | 1.00 | 37.32 | 7 |
| | ATOM | 1364 | CA | ARG | A | 438 | 20.534 | 51.379 | 33.821 | 1.00 | 39.30 | 6 |
| 55 | ATOM | 1365 | CB | ARG | A | 438 | 21.114 | 50.402 | 32.786 | 1.00 | 42.97 | 6 |
| | ATOM | 1366 | CG | ARG | A | 438 | 22.343 | 50.911 | 32.051 | 1.00 | 41.72 | 6 |
| | ATOM | 1367 | CD | ARG | A | 438 | 21.955 | 52.134 | 31.251 | 1.00 | 45.23 | 6 |
| | ATOM | 1368 | NE | ARG | A | 438 | 20.964 | 51.839 | 30.237 | 1.00 | 45.66 | 7 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| 5 | ATOM | 1369 | CZ | ARG | A | 438 | 20.063 | 52.718 | 30.318 | 1.00 | 50.91 | 6 |
| | ATOM | 1370 | NH1 | ARG | A | 438 | 20.046 | 53.958 | 30.318 | 1.00 | 50.91 | 7 |
| | ATOM | 1371 | NH2 | ARG | A | 438 | 19.198 | 52.354 | 28.865 | 1.00 | 46.86 | 7 |
| | ATOM | 1372 | C | ARG | A | 438 | 19.147 | 50.922 | 34.240 | 1.00 | 42.37 | 6 |
| | ATOM | 1373 | O | ARG | A | 438 | 18.147 | 51.297 | 33.625 | 1.00 | 40.58 | 8 |
| 10 | ATOM | 1374 | N | PHE | A | 439 | 19.080 | 50.120 | 35.298 | 1.00 | 42.25 | 7 |
| | ATOM | 1375 | CA | PHE | A | 439 | 17.803 | 49.624 | 35.763 | 1.00 | 42.81 | 6 |
| | ATOM | 1376 | CB | PHE | A | 439 | 17.975 | 48.794 | 37.013 | 1.00 | 42.18 | 6 |
| | ATOM | 1377 | CG | PHE | A | 439 | 16.739 | 48.053 | 37.413 | 1.00 | 42.48 | 6 |
| | ATOM | 1378 | CD1 | PHE | A | 439 | 16.198 | 47.111 | 36.562 | 1.00 | 47.09 | 6 |
| 15 | ATOM | 1379 | CD2 | PHE | A | 439 | 16.105 | 48.320 | 38.613 | 1.00 | 39.76 | 6 |
| | ATOM | 1380 | CE1 | PHE | A | 439 | 15.047 | 46.427 | 36.905 | 1.00 | 49.17 | 6 |
| | ATOM | 1381 | CE2 | PHE | A | 439 | 14.940 | 47.630 | 38.963 | 1.00 | 45.10 | 6 |
| | ATOM | 1382 | CZ | PHE | A | 439 | 14.411 | 46.683 | 38.098 | 1.00 | 46.36 | 6 |
| | ATOM | 1383 | C | PHE | A | 439 | 16.921 | 50.803 | 36.075 | 1.00 | 44.79 | 6 |
| 20 | ATOM | 1384 | O | PHE | A | 439 | 15.830 | 50.903 | 35.554 | 1.00 | 40.26 | 8 |
| | ATOM | 1385 | N | LEU | A | 440 | 17.410 | 51.681 | 36.951 | 1.00 | 42.77 | 7 |
| | ATOM | 1386 | CA | LEU | A | 440 | 16.660 | 52.871 | 37.344 | 1.00 | 42.96 | 6 |
| | ATOM | 1387 | CB | LEU | A | 440 | 17.546 | 53.824 | 38.150 | 1.00 | 37.19 | 6 |
| | ATOM | 1388 | CG | LEU | A | 440 | 17.943 | 53.297 | 39.500 | 1.00 | 36.97 | 6 |
| 25 | ATOM | 1389 | CD1 | LEU | A | 440 | 18.620 | 54.389 | 40.316 | 1.00 | 33.65 | 6 |
| | ATOM | 1390 | CD2 | LEU | A | 440 | 16.679 | 52.837 | 40.216 | 1.00 | 35.42 | 6 |
| | ATOM | 1391 | C | LEU | A | 440 | 16.025 | 53.596 | 36.168 | 1.00 | 45.47 | 6 |
| | ATOM | 1392 | O | LEU | A | 440 | 14.809 | 53.750 | 36.126 | 1.00 | 52.48 | 8 |
| | ATOM | 1393 | N | HIS | A | 441 | 16.836 | 54.060 | 35.223 | 1.00 | 49.15 | 7 |
| 30 | ATOM | 1394 | CA | HIS | A | 441 | 16.277 | 54.725 | 34.063 | 1.00 | 54.76 | 6 |
| | ATOM | 1395 | CB | HIS | A | 441 | 17.329 | 54.955 | 33.031 | 1.00 | 56.68 | 6 |
| | ATOM | 1396 | CG | HIS | A | 441 | 18.134 | 56.161 | 33.282 | 1.00 | 62.73 | 6 |
| | ATOM | 1397 | CD2 | HIS | A | 441 | 18.468 | 57.216 | 32.499 | 1.00 | 65.73 | 6 |
| | ATOM | 1398 | ND1 | HIS | A | 441 | 18.701 | 56.431 | 34.538 | 1.00 | 66.01 | 7 |
| 35 | ATOM | 1399 | CE1 | HIS | A | 441 | 19.332 | 57.594 | 34.473 | 1.00 | 65.55 | 6 |
| | ATOM | 1400 | NE2 | HIS | A | 441 | 19.205 | 58.085 | 33.255 | 1.00 | 60.09 | 7 |
| | ATOM | 1401 | C | HIS | A | 441 | 15.244 | 53.822 | 33.481 | 1.00 | 55.93 | 6 |
| | ATOM | 1402 | O | HIS | A | 441 | 14.149 | 54.263 | 33.170 | 1.00 | 57.33 | 8 |
| | ATOM | 1403 | N | MET | A | 442 | 15.605 | 52.549 | 33.313 | 1.00 | 57.81 | 7 |
| 40 | ATOM | 1404 | CA | MET | A | 442 | 14.661 | 51.583 | 32.778 | 1.00 | 59.11 | 6 |
| | ATOM | 1405 | CB | MET | A | 442 | 15.191 | 50.154 | 32.922 | 1.00 | 55.93 | 6 |
| | ATOM | 1406 | CG | MET | A | 442 | 16.336 | 49.813 | 32.022 | 1.00 | 58.52 | 6 |
| | ATOM | 1407 | SD | MET | A | 442 | 16.681 | 48.008 | 31.851 | 1.00 | 60.99 | 16 |
| | ATOM | 1408 | CE | MET | A | 442 | 17.085 | 47.602 | 33.581 | 1.00 | 52.61 | 6 |
| 45 | ATOM | 1409 | C | MET | A | 442 | 13.339 | 51.727 | 33.534 | 1.00 | 60.31 | 6 |
| | ATOM | 1410 | O | MET | A | 442 | 12.266 | 51.560 | 32.968 | 1.00 | 58.18 | 8 |
| | ATOM | 1411 | N | LYS | A | 443 | 13.425 | 52.054 | 34.818 | 1.00 | 61.45 | 7 |
| | ATOM | 1412 | CA | LYS | A | 443 | 12.236 | 52.202 | 35.626 | 1.00 | 64.90 | 6 |
| | ATOM | 1413 | CB | LYS | A | 443 | 12.608 | 52.141 | 37.090 | 1.00 | 64.40 | 6 |
| 50 | ATOM | 1414 | CG | LYS | A | 443 | 11.461 | 51.748 | 37.959 | 1.00 | 69.12 | 6 |
| | ATOM | 1415 | CD | LYS | A | 443 | 12.068 | 51.551 | 39.257 | 1.00 | 71.14 | 6 |
| | ATOM | 1416 | CE | LYS | A | 443 | 11.368 | 51.897 | 40.091 | 1.00 | 73.43 | 6 |
| | ATOM | 1417 | NZ | LYS | A | 443 | 11.883 | 51.712 | 41.415 | 1.00 | 67.97 | 7 |
| | ATOM | 1418 | C | LYS | A | 443 | 11.513 | 53.514 | 35.348 | 1.00 | 67.29 | 6 |
| 55 | ATOM | 1419 | O | LYS | A | 443 | 10.390 | 53.700 | 35.780 | 1.00 | 67.90 | 8 |
| | ATOM | 1420 | N | VAL | A | 444 | 12.171 | 54.429 | 34.629 | 1.00 | 66.57 | 7 |
| | ATOM | 1421 | CA | VAL | A | 444 | 11.575 | 55.719 | 34.297 | 1.00 | 64.76 | 6 |
| | ATOM | 1422 | CB | VAL | A | 444 | 12.569 | 56.869 | 34.560 | 1.00 | 62.76 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|----|
| 5 | ATOM | 1423 | CG1 | VAL | A | 444 | 11.952 | 58.195 | 34.174 | 1.00 | 61.089 | 6 |
| | ATOM | 1424 | CG2 | VAL | A | 444 | 12.999 | 56.891 | 36.035 | 1.00 | 59.27 | 6 |
| | ATOM | 1425 | C | VAL | A | 444 | 11.043 | 55.730 | 32.861 | 1.00 | 68.61 | 6 |
| | ATOM | 1426 | O | VAL | A | 444 | 9.937 | 56.210 | 32.612 | 1.00 | 70.60 | 8 |
| | ATOM | 1427 | N | GLU | A | 445 | 11.814 | 55.173 | 31.935 | 1.00 | 70.71 | 7 |
| 10 | ATOM | 1428 | CA | GLU | A | 445 | 11.457 | 55.152 | 30.514 | 1.00 | 71.45 | 6 |
| | ATOM | 1429 | CB | GLU | A | 445 | 12.725 | 55.255 | 29.664 | 1.00 | 72.36 | 6 |
| | ATOM | 1430 | CG | GLU | A | 445 | 13.598 | 56.429 | 30.022 | 1.00 | 40.00 | 6 |
| | ATOM | 1431 | CD | GLU | A | 445 | 14.875 | 56.472 | 29.239 | 1.00 | 40.00 | 6 |
| | ATOM | 1432 | OE1 | GLU | A | 445 | 15.155 | 55.565 | 28.414 | 1.00 | 40.00 | 8 |
| 15 | ATOM | 1433 | OE2 | GLU | A | 445 | 15.663 | 57.430 | 29.430 | 1.00 | 40.00 | 8 |
| | ATOM | 1434 | C | GLU | A | 445 | 10.724 | 53.912 | 30.049 | 1.00 | 71.46 | 6 |
| | ATOM | 1435 | O | GLU | A | 445 | 10.536 | 53.701 | 28.844 | 1.00 | 73.02 | 8 |
| | ATOM | 1436 | N | CYS | A | 446 | 10.301 | 53.099 | 30.999 | 1.00 | 71.12 | 7 |
| | ATOM | 1437 | CA | CYS | A | 446 | 9.628 | 51.899 | 30.634 | 1.00 | 70.83 | 6 |
| 20 | ATOM | 1438 | CB | CYS | A | 446 | 10.595 | 50.719 | 30.687 | 1.00 | 71.05 | 6 |
| | ATOM | 1439 | SG | CYS | A | 446 | 12.009 | 50.842 | 29.573 | 1.00 | 72.83 | 16 |
| | ATOM | 1440 | C | CYS | A | 446 | 8.454 | 51.671 | 31.535 | 1.00 | 71.91 | 6 |
| | ATOM | 1441 | O | CYS | A | 446 | 8.495 | 52.014 | 32.728 | 1.00 | 72.06 | 8 |
| | ATOM | 1442 | N | PRO | A | 447 | 7.372 | 51.133 | 30.978 | 1.00 | 73.12 | 7 |
| 25 | ATOM | 1443 | CD | PRO | A | 447 | 7.267 | 50.764 | 29.560 | 1.00 | 72.88 | 6 |
| | ATOM | 1444 | CA | PRO | A | 447 | 6.150 | 50.853 | 31.740 | 1.00 | 74.22 | 6 |
| | ATOM | 1445 | CB | PRO | A | 447 | 5.187 | 50.281 | 30.714 | 1.00 | 72.98 | 6 |
| | ATOM | 1446 | CG | PRO | A | 447 | 5.875 | 50.271 | 29.437 | 1.00 | 74.77 | 6 |
| | ATOM | 1447 | C | PRO | A | 447 | 6.435 | 49.843 | 32.831 | 1.00 | 75.94 | 6 |
| 30 | ATOM | 1448 | O | PRO | A | 447 | 7.181 | 48.908 | 32.612 | 1.00 | 76.67 | 8 |
| | ATOM | 1449 | N | THR | A | 448 | 5.820 | 50.002 | 33.997 | 1.00 | 76.91 | 7 |
| | ATOM | 1450 | CA | THR | A | 448 | 6.024 | 49.066 | 35.113 | 1.00 | 78.24 | 6 |
| | ATOM | 1451 | CB | THR | A | 448 | 5.528 | 49.734 | 36.401 | 1.00 | 81.33 | 6 |
| | ATOM | 1452 | OG1 | THR | A | 448 | 4.105 | 49.917 | 36.328 | 1.00 | 84.46 | 8 |
| 35 | ATOM | 1453 | CG2 | THR | A | 448 | 6.192 | 51.081 | 36.585 | 1.00 | 83.51 | 6 |
| | ATOM | 1454 | C | THR | A | 448 | 5.113 | 47.912 | 34.755 | 1.00 | 77.42 | 6 |
| | ATOM | 1455 | O | THR | A | 448 | 4.915 | 46.995 | 35.519 | 1.00 | 77.65 | 8 |
| | ATOM | 1456 | N | GLU | A | 449 | 4.539 | 48.021 | 33.565 | 1.00 | 76.29 | 7 |
| | ATOM | 1457 | CA | GLU | A | 449 | 3.630 | 47.023 | 33.024 | 1.00 | 75.03 | 6 |
| 40 | ATOM | 1458 | CB | GLU | A | 449 | 2.600 | 47.773 | 32.191 | 1.00 | 74.62 | 6 |
| | ATOM | 1459 | CG | GLU | A | 449 | 2.145 | 47.051 | 31.001 | 1.00 | 40.00 | 6 |
| | ATOM | 1460 | CD | GLU | A | 449 | 1.297 | 47.889 | 30.178 | 1.00 | 40.00 | 6 |
| | ATOM | 1461 | OE1 | GLU | A | 449 | 1.479 | 49.137 | 30.146 | 1.00 | 40.00 | 8 |
| | ATOM | 1462 | OE2 | GLU | A | 449 | 0.424 | 47.322 | 29.497 | 1.00 | 40.00 | 8 |
| 45 | ATOM | 1463 | C | GLU | A | 449 | 4.434 | 46.036 | 32.179 | 1.00 | 73.49 | 6 |
| | ATOM | 1464 | O | GLU | A | 449 | 3.882 | 45.142 | 31.559 | 1.00 | 70.24 | 8 |
| | ATOM | 1465 | N | LEU | A | 450 | 5.747 | 46.224 | 32.161 | 1.00 | 70.80 | 7 |
| | ATOM | 1466 | CA | LEU | A | 450 | 6.608 | 45.347 | 31.378 | 1.00 | 68.82 | 6 |
| | ATOM | 1467 | CB | LEU | A | 450 | 7.301 | 46.154 | 30.277 | 1.00 | 71.91 | 6 |
| 50 | ATOM | 1468 | CG | LEU | A | 450 | 6.464 | 46.819 | 29.217 | 1.00 | 76.62 | 6 |
| | ATOM | 1469 | CD1 | LEU | A | 450 | 7.337 | 47.662 | 28.328 | 1.00 | 77.95 | 6 |
| | ATOM | 1470 | CD2 | LEU | A | 450 | 5.786 | 45.750 | 28.415 | 1.00 | 76.46 | 6 |
| | ATOM | 1471 | C | LEU | A | 450 | 7.669 | 44.673 | 32.243 | 1.00 | 66.22 | 6 |
| | ATOM | 1472 | O | LEU | A | 450 | 8.427 | 43.841 | 31.752 | 1.00 | 66.01 | 8 |
| 55 | ATOM | 1473 | N | PHE | A | 451 | 7.705 | 45.039 | 33.530 | 1.00 | 61.96 | 7 |
| | ATOM | 1474 | CA | PHE | A | 451 | 8.681 | 44.506 | 34.480 | 1.00 | 58.44 | 6 |
| | ATOM | 1475 | CB | PHE | A | 451 | 9.041 | 45.562 | 35.540 | 1.00 | 61.34 | 6 |
| | ATOM | 1476 | CG | PHE | A | 451 | 9.873 | 46.717 | 35.008 | 1.00 | 63.02 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 1477 | CD1 | PHE | A | 451 | 9.426 | 47.507 | 33.963 | 1.00 | 62.92 | 6 |
| | ATOM | 1478 | CD2 | PHE | A | 451 | 11.089 | 47.017 | 35.593 | 1.00 | 63.07 | 6 |
| | ATOM | 1479 | CE1 | PHE | A | 451 | 10.199 | 48.598 | 33.521 | 1.00 | 65.12 | 6 |
| | ATOM | 1480 | CE2 | PHE | A | 451 | 11.860 | 48.102 | 35.156 | 1.00 | 64.66 | 6 |
| | ATOM | 1481 | CZ | PHE | A | 451 | 11.410 | 48.897 | 34.118 | 1.00 | 67.12 | 6 |
| 10 | ATOM | 1482 | C | PHE | A | 451 | 8.259 | 43.264 | 35.260 | 1.00 | 56.41 | 6 |
| | ATOM | 1483 | O | PHE | A | 451 | 7.641 | 43.392 | 36.331 | 1.00 | 56.56 | 8 |
| | ATOM | 1484 | N | PRO | A | 452 | 8.555 | 42.045 | 34.755 | 1.00 | 53.28 | 7 |
| | ATOM | 1485 | CD | PRO | A | 452 | 9.177 | 41.689 | 33.481 | 1.00 | 50.46 | 6 |
| | ATOM | 1486 | CA | PRO | A | 452 | 8.153 | 40.859 | 35.543 | 1.00 | 50.26 | 6 |
| 15 | ATOM | 1487 | CB | PRO | A | 452 | 8.739 | 39.680 | 34.780 | 1.00 | 49.19 | 6 |
| | ATOM | 1488 | CG | PRO | A | 452 | 9.178 | 40.206 | 33.482 | 1.00 | 45.89 | 6 |
| | ATOM | 1489 | C | PRO | A | 452 | 8.770 | 40.999 | 36.935 | 1.00 | 49.62 | 6 |
| | ATOM | 1490 | O | PRO | A | 452 | 9.867 | 41.529 | 37.094 | 1.00 | 52.35 | 8 |
| | ATOM | 1491 | N | PRO | A | 453 | 8.139 | 40.425 | 37.947 | 1.00 | 51.50 | 7 |
| 20 | ATOM | 1492 | CD | PRO | A | 453 | 7.001 | 39.542 | 37.797 | 1.00 | 49.66 | 6 |
| | ATOM | 1493 | CA | PRO | A | 453 | 8.610 | 40.528 | 39.323 | 1.00 | 50.89 | 6 |
| | ATOM | 1494 | CB | PRO | A | 453 | 7.675 | 39.659 | 40.109 | 1.00 | 51.49 | 6 |
| | ATOM | 1495 | CG | PRO | A | 453 | 6.703 | 39.141 | 39.185 | 1.00 | 50.82 | 6 |
| | ATOM | 1496 | C | PRO | A | 453 | 10.015 | 40.084 | 39.532 | 1.00 | 50.99 | 6 |
| 25 | ATOM | 1497 | O | PRO | A | 453 | 10.876 | 40.900 | 39.838 | 1.00 | 54.17 | 8 |
| | ATOM | 1498 | N | LEU | A | 454 | 10.255 | 38.781 | 39.423 | 1.00 | 51.21 | 7 |
| | ATOM | 1499 | CA | LEU | A | 454 | 11.585 | 38.298 | 39.674 | 1.00 | 47.17 | 6 |
| | ATOM | 1500 | CB | LEU | A | 454 | 11.813 | 36.962 | 38.975 | 1.00 | 44.44 | 6 |
| | ATOM | 1501 | CG | LEU | A | 454 | 13.167 | 36.375 | 39.289 | 1.00 | 41.33 | 6 |
| 30 | ATOM | 1502 | CD1 | LEU | A | 454 | 13.524 | 36.638 | 40.720 | 1.00 | 35.93 | 6 |
| | ATOM | 1503 | CD2 | LEU | A | 454 | 13.169 | 34.907 | 38.992 | 1.00 | 34.79 | 6 |
| | ATOM | 1504 | C | LEU | A | 454 | 12.541 | 39.375 | 39.182 | 1.00 | 42.25 | 6 |
| | ATOM | 1505 | O | LEU | A | 454 | 13.477 | 39.718 | 39.886 | 1.00 | 40.82 | 8 |
| | ATOM | 1506 | N | PHE | A | 455 | 12.270 | 39.957 | 38.011 | 1.00 | 39.29 | 7 |
| 35 | ATOM | 1507 | CA | PHE | A | 455 | 13.133 | 41.005 | 37.473 | 1.00 | 41.81 | 6 |
| | ATOM | 1508 | CB | PHE | A | 455 | 12.527 | 41.592 | 36.192 | 1.00 | 47.22 | 6 |
| | ATOM | 1509 | CG | PHE | A | 455 | 13.433 | 42.565 | 35.467 | 1.00 | 56.97 | 6 |
| | ATOM | 1510 | CD1 | PHE | A | 455 | 14.715 | 42.189 | 35.135 | 1.00 | 57.23 | 6 |
| | ATOM | 1511 | CD2 | PHE | A | 455 | 12.999 | 43.840 | 35.126 | 1.00 | 59.40 | 6 |
| 40 | ATOM | 1512 | CE1 | PHE | A | 455 | 15.557 | 43.059 | 34.466 | 1.00 | 56.58 | 6 |
| | ATOM | 1513 | CE2 | PHE | A | 455 | 13.848 | 44.716 | 34.452 | 1.00 | 61.80 | 6 |
| | ATOM | 1514 | CZ | PHE | A | 455 | 15.129 | 44.322 | 34.126 | 1.00 | 59.94 | 6 |
| | ATOM | 1515 | C | PHE | A | 455 | 13.273 | 42.085 | 38.534 | 1.00 | 45.12 | 6 |
| | ATOM | 1516 | O | PHE | A | 455 | 14.361 | 42.323 | 39.034 | 1.00 | 39.95 | 8 |
| 45 | ATOM | 1517 | N | LEU | A | 456 | 12.155 | 42.735 | 38.849 | 1.00 | 43.92 | 7 |
| | ATOM | 1518 | CA | LEU | A | 456 | 12.122 | 43.803 | 39.840 | 1.00 | 44.08 | 6 |
| | ATOM | 1519 | CB | LEU | A | 456 | 10.680 | 44.251 | 40.093 | 1.00 | 50.20 | 6 |
| | ATOM | 1520 | CG | LEU | A | 456 | 10.062 | 45.242 | 39.144 | 1.00 | 55.79 | 6 |
| | ATOM | 1521 | CD1 | LEU | A | 456 | 8.598 | 45.432 | 39.450 | 1.00 | 54.70 | 6 |
| 50 | ATOM | 1522 | CD2 | LEU | A | 456 | 10.807 | 46.548 | 39.295 | 1.00 | 53.01 | 6 |
| | ATOM | 1523 | C | LEU | A | 456 | 12.739 | 43.355 | 41.136 | 1.00 | 44.65 | 6 |
| | ATOM | 1524 | O | LEU | A | 456 | 13.597 | 44.022 | 41.685 | 1.00 | 45.93 | 8 |
| | ATOM | 1525 | N | GLU | A | 457 | 11.973 | 41.761 | 41.851 | 1.00 | 44.56 | 7 |
| | ATOM | 1526 | CA | GLU | A | 457 | 12.475 | 41.179 | 43.105 | 1.00 | 46.37 | 6 |
| 55 | ATOM | 1527 | C | GLU | A | 457 | 14.005 | 41.236 | 43.132 | 1.00 | 43.60 | 6 |
| | ATOM | 1528 | O | GLU | A | 457 | 14.583 | 41.724 | 44.117 | 1.00 | 42.69 | 8 |
| | ATOM | 1529 | CB | GLU | A | 457 | 12.024 | 39.723 | 43.223 | 1.00 | 50.16 | 6 |
| | ATOM | 1530 | CG | GLU | A | 457 | 11.114 | 39.476 | 44.427 | 1.00 | 20.00 | 6 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 1531 | CD | GLU | A | 457 | 10.807 | 37.994 | 44.848 | 1.00 | 20.00 | 6 |
| | ATOM | 1532 | OE1 | GLU | A | 457 | 11.673 | 37.099 | 44.311 | 1.00 | 20.00 | 8 |
| | ATOM | 1533 | OE2 | GLU | A | 457 | 9.683 | 37.639 | 45.172 | 1.00 | 20.00 | 8 |
| | ATOM | 1534 | N | VAL | A | 458 | 14.928 | 41.078 | 41.903 | 1.00 | 43.21 | 7 |
| | ATOM | 1535 | CA | VAL | A | 458 | 16.412 | 41.094 | 41.868 | 1.00 | 44.98 | 6 |
| 10 | ATOM | 1536 | CB | VAL | A | 458 | 16.881 | 40.306 | 40.642 | 1.00 | 44.83 | 6 |
| | ATOM | 1537 | CG1 | VAL | A | 458 | 18.365 | 40.106 | 40.698 | 1.00 | 49.72 | 6 |
| | ATOM | 1538 | CG2 | VAL | A | 458 | 16.185 | 38.979 | 40.558 | 1.00 | 40.89 | 6 |
| | ATOM | 1539 | C | VAL | A | 458 | 17.130 | 42.420 | 41.877 | 1.00 | 42.72 | 6 |
| | ATOM | 1540 | O | VAL | A | 458 | 18.061 | 42.617 | 42.658 | 1.00 | 42.88 | 8 |
| 15 | ATOM | 1541 | N | PHE | A | 459 | 16.713 | 43.325 | 41.010 | 1.00 | 44.53 | 7 |
| | ATOM | 1542 | CA | PHE | A | 459 | 17.385 | 44.606 | 40.892 | 1.00 | 48.18 | 6 |
| | ATOM | 1543 | CB | PHE | A | 459 | 17.281 | 45.104 | 39.494 | 1.00 | 43.60 | 6 |
| | ATOM | 1544 | CG | PHE | A | 459 | 17.915 | 44.190 | 38.547 | 1.00 | 40.79 | 6 |
| | ATOM | 1545 | CD1 | PHE | A | 459 | 17.325 | 42.983 | 38.244 | 1.00 | 41.01 | 6 |
| 20 | ATOM | 1546 | CD2 | PHE | A | 459 | 19.153 | 44.483 | 38.054 | 1.00 | 39.48 | 6 |
| | ATOM | 1547 | CE1 | PHE | A | 459 | 17.988 | 42.081 | 37.441 | 1.00 | 40.62 | 6 |
| | ATOM | 1548 | CE2 | PHE | A | 459 | 19.814 | 43.589 | 37.257 | 1.00 | 36.87 | 6 |
| | ATOM | 1549 | CZ | PHE | A | 459 | 19.233 | 42.385 | 36.940 | 1.00 | 36.39 | 6 |
| | ATOM | 1550 | C | PHE | A | 459 | 16.837 | 45.648 | 41.744 | 1.00 | 52.71 | 6 |
| 25 | ATOM | 1551 | O | PHE | A | 459 | 17.492 | 46.682 | 42.017 | 1.00 | 51.34 | 8 |
| | ATOM | 1552 | N | GLU | A | 460 | 15.606 | 45.422 | 42.161 | 1.00 | 62.92 | 7 |
| | ATOM | 1553 | CA | GLU | A | 460 | 15.066 | 46.428 | 42.965 | 1.00 | 69.33 | 6 |
| | ATOM | 1554 | CB | GLU | A | 460 | 13.552 | 46.352 | 43.094 | 1.00 | 72.95 | 6 |
| | ATOM | 1555 | CG | GLU | A | 460 | 12.978 | 47.767 | 42.957 | 1.00 | 78.35 | 6 |
| 30 | ATOM | 1556 | CD | GLU | A | 460 | 12.246 | 48.261 | 44.157 | 1.00 | 82.97 | 6 |
| | ATOM | 1557 | OE1 | GLU | A | 460 | 12.471 | 47.759 | 45.281 | 1.00 | 88.28 | 8 |
| | ATOM | 1558 | OE2 | GLU | A | 460 | 11.422 | 49.200 | 44.017 | 1.00 | 84.80 | 8 |
| | ATOM | 1559 | C | GLU | A | 460 | 15.736 | 46.245 | 44.272 | 1.00 | 71.87 | 6 |
| | ATOM | 1560 | O | GLU | A | 460 | 16.187 | 45.170 | 44.691 | 1.00 | 74.51 | 8 |
| 35 | ATOM | 1561 | N | ASP | A | 461 | 15.790 | 47.373 | 44.917 | 1.00 | 78.50 | 7 |
| | ATOM | 1562 | CA | ASP | A | 461 | 16.415 | 47.505 | 46.173 | 1.00 | 84.19 | 6 |
| | ATOM | 1563 | CB | ASP | A | 461 | 16.394 | 48.981 | 46.471 | 1.00 | 85.82 | 6 |
| | ATOM | 1564 | CG | ASP | A | 461 | 16.801 | 49.786 | 45.276 | 1.00 | 89.62 | 6 |
| | ATOM | 1565 | OD1 | ASP | A | 461 | 16.692 | 49.344 | 44.086 | 1.00 | 93.00 | 8 |
| 40 | ATOM | 1566 | OD2 | ASP | A | 461 | 17.239 | 50.923 | 45.482 | 1.00 | 93.04 | 8 |
| | ATOM | 1567 | C | ASP | A | 461 | 15.639 | 46.703 | 47.214 | 1.00 | 86.80 | 6 |
| | ATOM | 1568 | O | ASP | A | 461 | 16.245 | 45.748 | 47.731 | 1.00 | 88.70 | 8 |
| | ATOM | 1569 | OXT | ASP | A | 461 | 14.457 | 47.026 | 47.451 | 1.00 | 88.70 | 8 |
| | TER | | | | | | | | | | | |
| 45 | ATOM | 1 | CB | LYS | B | 211 | -20.802 | 66.251 | 39.780 | 1.00 | 46.72 | 6 |
| | ATOM | 2 | CG | LYS | B | 211 | -19.566 | 65.345 | 39.922 | 1.00 | 56.48 | 6 |
| | ATOM | 3 | CD | LYS | B | 211 | -18.264 | 66.114 | 40.045 | 1.00 | 60.93 | 6 |
| | ATOM | 4 | CE | LYS | B | 211 | -18.043 | 67.067 | 38.886 | 1.00 | 61.95 | 6 |
| | ATOM | 5 | NZ | LYS | B | 211 | -19.008 | 68.224 | 38.903 | 1.00 | 69.93 | 7 |
| 50 | ATOM | 6 | C | LYS | B | 211 | -22.418 | 67.861 | 40.818 | 1.00 | 35.68 | 6 |
| | ATOM | 7 | O | LYS | B | 211 | -23.356 | 67.113 | 40.454 | 1.00 | 33.58 | 8 |
| | ATOM | 8 | N | LYS | B | 211 | -20.742 | 66.675 | 42.239 | 1.00 | 45.76 | 7 |
| | ATOM | 9 | CA | LYS | B | 211 | -20.998 | 67.285 | 40.894 | 1.00 | 43.42 | 6 |
| | ATOM | 10 | N | PRO | B | 212 | -22.610 | 69.205 | 41.068 | 1.00 | 35.64 | 7 |
| 55 | ATOM | 11 | CD | PRO | B | 212 | -21.526 | 70.177 | 41.287 | 1.00 | 38.60 | 6 |
| | ATOM | 12 | CA | PRO | B | 212 | -23.943 | 69.861 | 41.036 | 1.00 | 38.35 | 6 |
| | ATOM | 13 | CB | PRO | B | 212 | -23.657 | 71.320 | 41.420 | 1.00 | 38.95 | 6 |
| | ATOM | 14 | CG | PRO | B | 212 | -22.226 | 71.474 | 41.551 | 1.00 | 42.00 | 6 |

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|----|------|----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 15 | C | PRO | B | 212 | -24.798 | 69.772 | 39.807 | 1.00 | 38.78 | 6 |
| | ATOM | 16 | O | PRO | B | 212 | -24.350 | 70.045 | 38.696 | 1.00 | 34.64 | 8 |
| | ATOM | 17 | N | GLU | B | 213 | -26.058 | 69.424 | 40.032 | 1.00 | 40.31 | 7 |
| | ATOM | 18 | CA | GLU | B | 213 | -27.081 | 69.290 | 39.003 | 1.00 | 43.87 | 6 |
| | ATOM | 19 | CB | GLU | B | 213 | -27.895 | 68.004 | 39.265 | 1.00 | 45.16 | 6 |
| 10 | ATOM | 20 | CG | GLU | B | 213 | -27.032 | 66.709 | 39.286 | 1.00 | 47.60 | 6 |
| | ATOM | 21 | CD | GLU | B | 213 | -27.807 | 65.421 | 39.199 | 1.00 | 50.68 | 6 |
| | ATOM | 22 | OE1 | GLU | B | 213 | -28.847 | 65.244 | 39.886 | 1.00 | 59.18 | 8 |
| | ATOM | 23 | OE2 | GLU | B | 213 | -27.382 | 64.516 | 38.442 | 1.00 | 49.06 | 8 |
| | ATOM | 24 | C | GLU | B | 213 | -27.924 | 70.576 | 39.080 | 1.00 | 45.96 | 6 |
| 15 | ATOM | 25 | O | GLU | B | 213 | -27.624 | 71.467 | 39.859 | 1.00 | 43.13 | 8 |
| | ATOM | 26 | N | PRO | B | 214 | -28.987 | 70.698 | 38.308 | 1.00 | 46.52 | 7 |
| | ATOM | 27 | CD | PRO | B | 214 | -29.484 | 69.635 | 37.446 | 1.00 | 46.44 | 6 |
| | ATOM | 28 | CA | PRO | B | 214 | -29.843 | 71.907 | 38.302 | 1.00 | 47.52 | 6 |
| | ATOM | 29 | CB | PRO | B | 214 | -30.799 | 71.639 | 37.210 | 1.00 | 45.40 | 6 |
| 20 | ATOM | 30 | CG | PRO | B | 214 | -30.530 | 70.257 | 36.805 | 1.00 | 49.89 | 6 |
| | ATOM | 31 | C | PRO | B | 214 | -30.574 | 72.330 | 39.535 | 1.00 | 45.70 | 6 |
| | ATOM | 32 | O | PRO | B | 214 | -30.597 | 71.595 | 40.483 | 1.00 | 44.49 | 8 |
| | ATOM | 33 | N | THR | B | 215 | -31.180 | 73.515 | 39.506 | 1.00 | 45.24 | 7 |
| | ATOM | 34 | CA | THR | B | 215 | -31.965 | 74.036 | 40.652 | 1.00 | 49.36 | 6 |
| 25 | ATOM | 35 | CB | THR | B | 215 | -31.443 | 75.420 | 41.091 | 1.00 | 44.86 | 6 |
| | ATOM | 36 | OG1 | THR | B | 215 | -32.249 | 76.464 | 40.534 | 1.00 | 52.26 | 8 |
| | ATOM | 37 | CG2 | THR | B | 215 | -30.011 | 75.617 | 40.659 | 1.00 | 39.43 | 6 |
| | ATOM | 38 | C | THR | B | 215 | -33.386 | 74.239 | 40.114 | 1.00 | 52.51 | 6 |
| | ATOM | 39 | O | THR | B | 215 | -33.562 | 74.868 | 39.078 | 1.00 | 53.48 | 8 |
| 30 | ATOM | 40 | N | ASP | B | 216 | -34.387 | 73.741 | 40.829 | 1.00 | 58.81 | 7 |
| | ATOM | 41 | CA | ASP | B | 216 | -35.795 | 73.865 | 40.435 | 1.00 | 61.51 | 6 |
| | ATOM | 42 | CB | ASP | B | 216 | -36.674 | 74.005 | 41.650 | 1.00 | 70.57 | 6 |
| | ATOM | 43 | CG | ASP | B | 216 | -37.675 | 72.981 | 41.710 | 1.00 | 78.07 | 6 |
| | ATOM | 44 | OD1 | ASP | B | 216 | -38.228 | 72.588 | 40.652 | 1.00 | 82.31 | 8 |
| 35 | ATOM | 45 | OD2 | ASP | B | 216 | -37.983 | 72.567 | 42.830 | 1.00 | 86.55 | 8 |
| | ATOM | 46 | C | ASP | B | 216 | -35.920 | 75.123 | 39.648 | 1.00 | 58.42 | 6 |
| | ATOM | 47 | O | ASP | B | 216 | -36.847 | 75.317 | 38.827 | 1.00 | 56.85 | 8 |
| | ATOM | 48 | N | GLU | B | 217 | -34.954 | 75.979 | 39.984 | 1.00 | 54.92 | 7 |
| | ATOM | 49 | CA | GLU | B | 217 | -34.851 | 77.259 | 39.353 | 1.00 | 53.37 | 6 |
| 40 | ATOM | 50 | CB | GLU | B | 217 | -34.104 | 78.264 | 40.251 | 1.00 | 51.02 | 6 |
| | ATOM | 51 | CG | GLU | B | 217 | -34.151 | 79.689 | 39.679 | 1.00 | 40.00 | 6 |
| | ATOM | 52 | CD | GLU | B | 217 | -34.301 | 80.745 | 40.739 | 1.00 | 40.00 | 6 |
| | ATOM | 53 | OE1 | GLU | B | 217 | -34.089 | 80.443 | 41.945 | 1.00 | 40.00 | 8 |
| | ATOM | 54 | OE2 | GLU | B | 217 | -34.625 | 81.921 | 40.411 | 1.00 | 40.00 | 8 |
| 45 | ATOM | 55 | C | GLU | B | 217 | -34.232 | 77.163 | 37.957 | 1.00 | 53.55 | 6 |
| | ATOM | 56 | O | GLU | B | 217 | -34.815 | 77.612 | 37.018 | 1.00 | 54.33 | 8 |
| | ATOM | 57 | N | GLU | B | 218 | -33.063 | 76.572 | 37.839 | 1.00 | 49.20 | 7 |
| | ATOM | 58 | CA | GLU | B | 218 | -32.318 | 76.385 | 36.608 | 1.00 | 45.94 | 6 |
| | ATOM | 59 | CB | GLU | B | 218 | -30.965 | 75.793 | 36.981 | 1.00 | 43.43 | 6 |
| 50 | ATOM | 60 | CG | GLU | B | 218 | -30.065 | 76.728 | 37.801 | 1.00 | 40.86 | 6 |
| | ATOM | 61 | CD | GLU | B | 218 | -28.713 | 76.159 | 38.072 | 1.00 | 39.88 | 6 |
| | ATOM | 62 | OE1 | GLU | B | 218 | -28.606 | 74.967 | 38.449 | 1.00 | 37.61 | 8 |
| | ATOM | 63 | OE2 | GLU | B | 218 | -27.707 | 76.901 | 37.945 | 1.00 | 34.01 | 8 |
| | ATOM | 64 | C | GLU | B | 218 | -33.014 | 75.475 | 35.610 | 1.00 | 44.71 | 6 |
| 55 | ATOM | 65 | O | GLU | B | 218 | -32.935 | 75.686 | 34.405 | 1.00 | 45.31 | 8 |
| | ATOM | 66 | N | TRP | B | 219 | -33.669 | 74.439 | 36.131 | 1.00 | 44.02 | 7 |
| | ATOM | 67 | CA | TRP | B | 219 | -34.368 | 73.490 | 35.290 | 1.00 | 46.97 | 6 |
| | ATOM | 68 | CB | TRP | B | 219 | -35.046 | 72.408 | 36.119 | 1.00 | 48.42 | 6 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 69 | CG | TRP | B | 219 | -34.195 | 71.230 | 36.374 | 1.00 | 54.61 | 6 |
| | ATOM | 70 | CD2 | TRP | B | 219 | -34.048 | 70.120 | 35.478 | 1.00 | 55.24 | 6 |
| | ATOM | 71 | CE2 | TRP | B | 219 | -33.076 | 69.248 | 36.063 | 1.00 | 53.67 | 6 |
| | ATOM | 72 | CE3 | TRP | B | 219 | -34.615 | 69.771 | 34.252 | 1.00 | 54.55 | 6 |
| | ATOM | 73 | CD1 | TRP | B | 219 | -33.399 | 71.019 | 37.415 | 1.00 | 55.75 | 6 |
| 10 | ATOM | 74 | NE1 | TRP | B | 219 | -32.697 | 69.838 | 37.236 | 1.00 | 54.43 | 7 |
| | ATOM | 75 | CZ2 | TRP | B | 219 | -32.635 | 68.075 | 35.431 | 1.00 | 52.54 | 6 |
| | ATOM | 76 | CZ3 | TRP | B | 219 | -34.214 | 68.603 | 33.643 | 1.00 | 55.17 | 6 |
| | ATOM | 77 | CH2 | TRP | B | 219 | -33.234 | 67.758 | 34.214 | 1.00 | 55.59 | 6 |
| | ATOM | 78 | C | TRP | B | 219 | -35.409 | 74.199 | 34.459 | 1.00 | 47.32 | 6 |
| 15 | ATOM | 79 | O | TRP | B | 219 | -35.561 | 73.914 | 33.277 | 1.00 | 43.56 | 8 |
| | ATOM | 80 | N | GLU | B | 220 | -36.126 | 75.130 | 35.084 | 1.00 | 49.91 | 7 |
| | ATOM | 81 | CA | GLU | B | 220 | -37.158 | 75.874 | 34.402 | 1.00 | 53.57 | 6 |
| | ATOM | 82 | CB | GLU | B | 220 | -37.811 | 76.820 | 35.373 | 1.00 | 58.18 | 6 |
| | ATOM | 83 | CG | GLU | B | 220 | -39.251 | 76.812 | 35.221 | 1.00 | 73.13 | 6 |
| 20 | ATOM | 84 | CD | GLU | B | 220 | -39.824 | 76.858 | 36.489 | 1.00 | 80.06 | 6 |
| | ATOM | 85 | OE1 | GLU | B | 220 | -39.485 | 75.995 | 37.324 | 1.00 | 82.12 | 8 |
| | ATOM | 86 | OE2 | GLU | B | 220 | -40.635 | 77.740 | 36.718 | 1.00 | 82.78 | 8 |
| | ATOM | 87 | C | GLU | B | 220 | -36.539 | 76.645 | 33.250 | 1.00 | 50.51 | 6 |
| | ATOM | 88 | O | GLU | B | 220 | -37.160 | 76.793 | 32.195 | 1.00 | 49.94 | 8 |
| 25 | ATOM | 89 | N | LEU | B | 221 | -35.312 | 77.135 | 33.455 | 1.00 | 43.71 | 7 |
| | ATOM | 90 | CA | LEU | B | 221 | -34.604 | 77.884 | 32.411 | 1.00 | 42.81 | 6 |
| | ATOM | 91 | CB | LEU | B | 221 | -33.214 | 78.324 | 32.865 | 1.00 | 39.21 | 6 |
| | ATOM | 92 | CG | LEU | B | 221 | -32.321 | 78.833 | 31.754 | 1.00 | 36.34 | 6 |
| | ATOM | 93 | CD1 | LEU | B | 221 | -33.073 | 79.843 | 30.927 | 1.00 | 36.93 | 6 |
| 30 | ATOM | 94 | CD2 | LEU | B | 221 | -31.058 | 79.446 | 32.331 | 1.00 | 24.18 | 6 |
| | ATOM | 95 | C | LEU | B | 221 | -34.454 | 77.011 | 31.192 | 1.00 | 43.46 | 6 |
| | ATOM | 96 | O | LEU | B | 221 | -34.819 | 77.406 | 30.104 | 1.00 | 45.25 | 8 |
| | ATOM | 97 | N | ILE | B | 222 | -33.878 | 75.829 | 31.398 | 1.00 | 39.09 | 7 |
| | ATOM | 98 | CA | ILE | B | 222 | -33.687 | 74.857 | 30.330 | 1.00 | 35.47 | 6 |
| 35 | ATOM | 99 | CB | ILE | B | 222 | -33.224 | 73.516 | 30.871 | 1.00 | 33.74 | 6 |
| | ATOM | 100 | CG2 | ILE | B | 222 | -33.204 | 72.488 | 29.776 | 1.00 | 28.86 | 6 |
| | ATOM | 101 | CG1 | ILE | B | 222 | -31.840 | 73.631 | 31.493 | 1.00 | 33.33 | 6 |
| | ATOM | 102 | CD1 | ILE | B | 222 | -31.435 | 72.419 | 32.264 | 1.00 | 34.85 | 6 |
| | ATOM | 103 | C | ILE | B | 222 | -34.991 | 74.627 | 29.598 | 1.00 | 34.26 | 6 |
| 40 | ATOM | 104 | O | ILE | B | 222 | -35.082 | 74.832 | 28.392 | 1.00 | 31.90 | 8 |
| | ATOM | 105 | N | LYS | B | 223 | -35.992 | 74.183 | 30.346 | 1.00 | 39.49 | 7 |
| | ATOM | 106 | CA | LYS | B | 223 | -37.300 | 73.892 | 29.785 | 1.00 | 44.43 | 6 |
| | ATOM | 107 | CB | LYS | B | 223 | -38.351 | 73.876 | 30.882 | 1.00 | 50.81 | 6 |
| | ATOM | 108 | CG | LYS | B | 223 | -39.693 | 73.358 | 30.411 | 1.00 | 62.51 | 6 |
| 45 | ATOM | 109 | CD | LYS | B | 223 | -40.795 | 73.532 | 31.449 | 1.00 | 72.22 | 6 |
| | ATOM | 110 | CE | LYS | B | 223 | -42.163 | 73.249 | 30.827 | 1.00 | 74.55 | 6 |
| | ATOM | 111 | NZ | LYS | B | 223 | -43.268 | 73.378 | 31.837 | 1.00 | 75.78 | 7 |
| | ATOM | 112 | C | LYS | B | 223 | -37.648 | 74.942 | 28.755 | 1.00 | 42.81 | 6 |
| | ATOM | 113 | O | LYS | B | 223 | -38.337 | 74.661 | 27.796 | 1.00 | 40.36 | 8 |
| 50 | ATOM | 114 | N | THR | B | 224 | -37.146 | 76.156 | 28.979 | 1.00 | 39.89 | 7 |
| | ATOM | 115 | CA | THR | B | 224 | -37.353 | 77.293 | 28.074 | 1.00 | 39.93 | 6 |
| | ATOM | 116 | CB | THR | B | 224 | -36.956 | 78.609 | 28.776 | 1.00 | 40.57 | 6 |
| | ATOM | 117 | OG1 | THR | B | 224 | -37.646 | 78.740 | 30.028 | 1.00 | 39.27 | 8 |
| | ATOM | 118 | CG2 | THR | B | 224 | -37.273 | 79.805 | 27.893 | 1.00 | 38.11 | 6 |
| 55 | ATOM | 119 | C | THR | B | 224 | -36.521 | 77.094 | 26.789 | 1.00 | 39.96 | 6 |
| | ATOM | 120 | O | THR | B | 224 | -37.043 | 76.677 | 25.756 | 1.00 | 36.67 | 8 |
| | ATOM | 121 | N | VAL | B | 225 | -35.231 | 77.421 | 26.888 | 1.00 | 38.02 | 7 |
| | ATOM | 122 | CA | VAL | B | 225 | -34.263 | 77.295 | 25.801 | 1.00 | 38.12 | 6 |

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|----|------|-----|-----|-----|---|-----|---------|--------|-------------------|------|-------------------|--------------|
| 5 | ATOM | 123 | CB | VAL | B | 225 | -32.869 | 77.015 | 28.848 | 1.00 | 38.193 | 6 |
| | ATOM | 124 | CG1 | VAL | B | 225 | -31.863 | 76.983 | 25.226 | 1.00 | 36.77 | 6 |
| | ATOM | 125 | CG2 | VAL | B | 225 | -32.483 | 78.050 | 27.353 | 1.00 | 41.76 | 6 |
| | ATOM | 126 | C | VAL | B | 225 | -34.656 | 76.191 | 24.843 | 1.00 | 37.52 | 6 |
| | ATOM | 127 | O | VAL | B | 225 | -34.621 | 76.364 | 23.638 | 1.00 | 36.77 | 8 |
| 10 | ATOM | 128 | N | THR | B | 226 | -35.005 | 75.046 | 25.410 | 1.00 | 34.02 | 7 |
| | ATOM | 129 | CA | THR | B | 226 | -35.423 | 73.887 | 24.638 | 1.00 | 34.67 | 6 |
| | ATOM | 130 | CB | THR | B | 226 | -35.677 | 72.707 | 25.574 | 1.00 | 30.56 | 6 |
| | ATOM | 131 | OG1 | THR | B | 226 | -34.432 | 72.225 | 26.084 | 1.00 | 32.20 | 8 |
| | ATOM | 132 | CG2 | THR | B | 226 | -36.413 | 71.595 | 24.874 | 1.00 | 20.99 | 6 |
| 15 | ATOM | 133 | C | THR | B | 226 | -36.664 | 74.170 | 23.803 | 1.00 | 36.41 | 6 |
| | ATOM | 134 | O | THR | B | 226 | -36.633 | 74.054 | 22.578 | 1.00 | 39.64 | 8 |
| | ATOM | 135 | N | ALA | B | 227 | -37.746 | 74.542 | 24.480 | 1.00 | 39.20 | 7 |
| | ATOM | 136 | CA | ALA | B | 227 | -39.008 | 74.861 | 23.822 | 1.00 | 36.93 | 6 |
| | ATOM | 137 | CB | ALA | B | 227 | -39.914 | 75.631 | 24.785 | 1.00 | 38.06 | 6 |
| 20 | ATOM | 138 | C | ALA | B | 227 | -38.686 | 75.719 | 22.608 | 1.00 | 37.69 | 6 |
| | ATOM | 139 | O | ALA | B | 227 | -39.317 | 75.616 | 21.566 | 1.00 | 40.94 | 8 |
| | ATOM | 140 | N | ALA | B | 228 | -37.677 | 76.572 | 22.785 | 1.00 | 32.86 | 7 |
| | ATOM | 141 | CA | ALA | B | 228 | -37.216 | 77.483 | 21.753 | 1.00 | 32.48 | 6 |
| | ATOM | 142 | CB | ALA | B | 228 | -36.252 | 78.458 | 22.358 | 1.00 | 28.25 | 6 |
| 25 | ATOM | 143 | C | ALA | B | 228 | -36.545 | 76.704 | 20.638 | 1.00 | 36.12 | 6 |
| | ATOM | 144 | O | ALA | B | 228 | -37.078 | 76.586 | 19.544 | 1.00 | 37.86 | 8 |
| | ATOM | 145 | N | HIS | B | 229 | -35.364 | 76.175 | 20.924 | 1.00 | 33.58 | 7 |
| | ATOM | 146 | CA | HIS | B | 229 | -34.611 | 75.409 | 19.956 | 1.00 | 32.97 | 6 |
| | ATOM | 147 | CB | HIS | B | 229 | -33.418 | 74.721 | 20.597 | 1.00 | 33.69 | 6 |
| 30 | ATOM | 148 | CG | HIS | B | 229 | -32.776 | 73.714 | 19.715 | 1.00 | 28.39 | 6 |
| | ATOM | 149 | CD2 | HIS | B | 229 | -32.535 | 72.384 | 19.863 | 1.00 | 28.83 | 6 |
| | ATOM | 150 | ND1 | HIS | B | 229 | -32.336 | 74.030 | 18.426 | 1.00 | 30.47 | 7 |
| | ATOM | 151 | CE1 | HIS | B | 229 | -31.867 | 72.929 | 17.855 | 1.00 | 26.95 | 6 |
| | ATOM | 152 | NE2 | HIS | B | 229 | -31.976 | 71.927 | 18.700 | 1.00 | 31.27 | 7 |
| 35 | ATOM | 153 | C | HIS | B | 229 | -35.362 | 74.352 | 19.202 | 1.00 | 38.40 | 6 |
| | ATOM | 154 | O | HIS | B | 229 | -35.069 | 74.131 | 18.045 | 1.00 | 41.49 | 8 |
| | ATOM | 155 | N | VAL | B | 230 | -36.296 | 73.688 | 19.882 | 1.00 | 38.55 | 7 |
| | ATOM | 156 | CA | VAL | B | 230 | -37.077 | 72.634 | 19.263 | 1.00 | 40.40 | 6 |
| | ATOM | 157 | CB | VAL | B | 230 | -37.744 | 71.747 | 20.310 | 1.00 | 44.68 | 6 |
| 40 | ATOM | 158 | CG1 | VAL | B | 230 | -38.381 | 70.537 | 19.637 | 1.00 | 39.39 | 6 |
| | ATOM | 159 | CG2 | VAL | B | 230 | -36.742 | 71.311 | 21.356 | 1.00 | 42.18 | 6 |
| | ATOM | 160 | C | VAL | B | 230 | -38.133 | 73.130 | 18.284 | 1.00 | 44.28 | 6 |
| | ATOM | 161 | O | VAL | B | 230 | -38.375 | 72.505 | 17.248 | 1.00 | 45.94 | 8 |
| | ATOM | 162 | N | ALA | B | 231 | -38.774 | 74.240 | 18.623 | 1.00 | 45.59 | 7 |
| 45 | ATOM | 163 | CA | ALA | B | 231 | -39.820 | 74.804 | 17.792 | 1.00 | 47.84 | 6 |
| | ATOM | 164 | CB | ALA | B | 231 | -40.736 | 75.661 | 18.647 | 1.00 | 45.08 | 6 |
| | ATOM | 165 | C | ALA | B | 231 | -39.235 | 75.636 | 16.673 | 1.00 | 48.04 | 6 |
| | ATOM | 166 | O | ALA | B | 231 | -39.959 | 76.128 | 15.816 | 1.00 | 49.95 | 8 |
| | ATOM | 167 | N | THR | B | 232 | -37.914 | 75.773 | 16.669 | 1.00 | 47.26 | 7 |
| 50 | ATOM | 168 | CA | THR | B | 232 | -37.220 | 76.563 | 15.654 | 1.00 | 43.64 | 6 |
| | ATOM | 169 | CB | THR | B | 232 | -36.482 | 77.746 | 16.315 | 1.00 | 41.93 | 6 |
| | ATOM | 170 | OG1 | THR | B | 232 | -35.385 | 77.270 | 17.098 | 1.00 | 39.10 | 8 |
| | ATOM | 171 | CG2 | THR | B | 232 | -37.423 | 78.523 | 17.232 | 1.00 | 29.80 | 6 |
| | ATOM | 172 | C | THR | B | 232 | -36.194 | 75.719 | 14.914 | 1.00 | 43.97 | 6 |
| 55 | ATOM | 173 | O | THR | B | 232 | -35.401 | 76.252 | 14.155 | 1.00 | 40.55 | 8 |
| | ATOM | 174 | N | ASN | B | 233 | -36.195 | 74.407 | 15.157 | 1.00 | 48.62 | 7 |
| | ATOM | 175 | CA | ASN | B | 233 | -35.247 | 73.511 | 14.483 | 1.00 | 58.62 | 6 |
| | ATOM | 176 | CB | ASN | B | 233 | -34.621 | 72.537 | 15.500 | 1.00 | 62.44 | 6 |

| | | | | | | | | | | | | |
|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 177 | CG | ASN | B | 233 | -33.407 | 71.812 | 14.943 | 1.00 | 68.33 | 6 |
| | ATOM | 178 | OD1 | ASN | B | 233 | -32.569 | 72.427 | 14.256 | 1.00 | 65.50 | 8 |
| | ATOM | 179 | ND2 | ASN | B | 233 | -33.288 | 70.529 | 15.265 | 1.00 | 74.29 | 7 |
| | ATOM | 180 | C | ASN | B | 233 | -36.033 | 72.755 | 13.437 | 1.00 | 65.06 | 6 |
| | ATOM | 181 | O | ASN | B | 233 | -36.950 | 72.005 | 13.754 | 1.00 | 69.47 | 8 |
| 10 | ATOM | 182 | N | ALA | B | 234 | -35.674 | 72.986 | 12.182 | 1.00 | 68.80 | 7 |
| | ATOM | 183 | CA | ALA | B | 234 | -36.352 | 72.376 | 11.036 | 1.00 | 70.98 | 6 |
| | ATOM | 184 | CB | ALA | B | 234 | -35.585 | 72.701 | 9.769 | 1.00 | 71.43 | 6 |
| | ATOM | 185 | C | ALA | B | 234 | -36.556 | 70.880 | 11.111 | 1.00 | 73.83 | 6 |
| | ATOM | 186 | O | ALA | B | 234 | -35.677 | 70.142 | 11.501 | 1.00 | 74.33 | 8 |
| 15 | ATOM | 187 | N | GLN | B | 235 | -37.754 | 70.479 | 10.717 | 1.00 | 75.07 | 7 |
| | ATOM | 188 | CA | GLN | B | 235 | -38.149 | 69.095 | 10.690 | 1.00 | 76.32 | 6 |
| | ATOM | 189 | CB | GLN | B | 235 | -37.468 | 68.365 | 9.533 | 1.00 | 76.98 | 6 |
| | ATOM | 190 | CG | GLN | B | 235 | -38.120 | 68.540 | 8.170 | 1.00 | 77.07 | 6 |
| | ATOM | 191 | CD | GLN | B | 235 | -38.572 | 69.940 | 7.909 | 1.00 | 80.85 | 6 |
| 20 | ATOM | 192 | OE1 | GLN | B | 235 | -39.575 | 70.401 | 8.491 | 1.00 | 82.01 | 8 |
| | ATOM | 193 | NE2 | GLN | B | 235 | -37.862 | 70.620 | 7.040 | 1.00 | 78.80 | 7 |
| | ATOM | 194 | C | GLN | B | 235 | -37.904 | 68.331 | 11.953 | 1.00 | 77.15 | 6 |
| | ATOM | 195 | O | GLN | B | 235 | -38.087 | 67.137 | 11.947 | 1.00 | 76.06 | 8 |
| | ATOM | 196 | N | GLY | B | 236 | -37.511 | 68.985 | 13.039 | 1.00 | 77.46 | 7 |
| 25 | ATOM | 197 | CA | GLY | B | 236 | -37.304 | 68.263 | 14.288 | 1.00 | 78.37 | 6 |
| | ATOM | 198 | C | GLY | B | 236 | -36.717 | 66.882 | 14.217 | 1.00 | 79.43 | 6 |
| | ATOM | 199 | O | GLY | B | 236 | -35.717 | 66.650 | 13.542 | 1.00 | 79.47 | 8 |
| | ATOM | 200 | N | SER | B | 237 | -37.420 | 66.007 | 14.943 | 1.00 | 77.98 | 7 |
| | ATOM | 201 | CA | SER | B | 237 | -37.117 | 64.600 | 15.092 | 1.00 | 76.49 | 6 |
| 30 | ATOM | 202 | CB | SER | B | 237 | -38.118 | 63.953 | 16.066 | 1.00 | 76.46 | 6 |
| | ATOM | 203 | C | SER | B | 237 | -37.181 | 63.895 | 13.737 | 1.00 | 75.35 | 6 |
| | ATOM | 204 | O | SER | B | 237 | -36.493 | 62.911 | 13.524 | 1.00 | 75.47 | 8 |
| | ATOM | 205 | N | HIS | B | 238 | -38.004 | 64.443 | 12.845 | 1.00 | 75.56 | 7 |
| | ATOM | 206 | CA | HIS | B | 238 | -38.293 | 63.926 | 11.519 | 1.00 | 75.46 | 6 |
| 35 | ATOM | 207 | CB | HIS | B | 238 | -39.663 | 64.397 | 11.096 | 1.00 | 75.85 | 6 |
| | ATOM | 208 | C | HIS | B | 238 | -37.369 | 64.216 | 10.380 | 1.00 | 74.10 | 6 |
| | ATOM | 209 | O | HIS | B | 238 | -37.747 | 64.135 | 9.222 | 1.00 | 75.34 | 8 |
| | ATOM | 210 | N | TRP | B | 239 | -36.127 | 64.427 | 10.651 | 1.00 | 73.39 | 7 |
| | ATOM | 211 | CA | TRP | B | 239 | -35.345 | 64.786 | 9.519 | 1.00 | 74.02 | 6 |
| 40 | ATOM | 212 | CB | TRP | B | 239 | -34.121 | 65.542 | 9.934 | 1.00 | 81.77 | 6 |
| | ATOM | 213 | CG | TRP | B | 239 | -33.085 | 64.786 | 10.737 | 1.00 | 89.67 | 6 |
| | ATOM | 214 | CD2 | TRP | B | 239 | -31.727 | 64.530 | 10.302 | 1.00 | 93.19 | 6 |
| | ATOM | 215 | CE2 | TRP | B | 239 | -31.069 | 63.848 | 11.393 | 1.00 | 95.46 | 6 |
| | ATOM | 216 | CE3 | TRP | B | 239 | -30.949 | 64.941 | 9.196 | 1.00 | 95.35 | 6 |
| 45 | ATOM | 217 | CD1 | TRP | B | 239 | -33.237 | 64.180 | 11.926 | 1.00 | 94.16 | 6 |
| | ATOM | 218 | NE1 | TRP | B | 239 | -32.022 | 63.631 | 12.347 | 1.00 | 97.48 | 7 |
| | ATOM | 219 | CZ2 | TRP | B | 239 | -29.706 | 63.475 | 11.348 | 1.00 | 96.23 | 6 |
| | ATOM | 220 | CZ3 | TRP | B | 239 | -29.613 | 64.533 | 9.128 | 1.00 | 96.75 | 6 |
| | ATOM | 221 | CH2 | TRP | B | 239 | -28.978 | 63.870 | 10.215 | 1.00 | 97.32 | 6 |
| 50 | ATOM | 222 | C | TRP | B | 239 | -34.994 | 63.722 | 8.539 | 1.00 | 70.77 | 6 |
| | ATOM | 223 | O | TRP | B | 239 | -35.423 | 63.772 | 7.388 | 1.00 | 71.70 | 8 |
| | ATOM | 224 | N | LYS | B | 240 | -34.165 | 62.791 | 8.955 | 1.00 | 67.10 | 7 |
| | ATOM | 225 | CA | LYS | B | 240 | -33.724 | 61.744 | 8.077 | 1.00 | 65.63 | 6 |
| | ATOM | 226 | CB | LYS | B | 240 | -33.321 | 60.539 | 8.906 | 1.00 | 66.65 | 6 |
| 55 | ATOM | 227 | CG | LYS | B | 240 | -32.210 | 60.824 | 9.905 | 1.00 | 69.83 | 6 |
| | ATOM | 228 | CD | LYS | B | 240 | -31.759 | 59.553 | 10.602 | 1.00 | 71.49 | 6 |
| | ATOM | 229 | CE | LYS | B | 240 | -30.576 | 59.843 | 11.493 | 1.00 | 71.31 | 6 |
| | ATOM | 230 | NZ | LYS | B | 240 | -30.106 | 58.604 | 12.157 | 1.00 | 72.23 | 7 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 231 | C | LYS | B | 240 | -34.719 | 61.331 | 6.996 | 1.00 | 66.19 | 6 |
| | ATOM | 232 | O | LYS | B | 240 | -34.321 | 60.673 | 6.031 | 1.00 | 65.20 | 8 |
| | ATOM | 233 | N | ASN | B | 241 | -35.986 | 61.727 | 7.139 | 1.00 | 66.69 | 7 |
| | ATOM | 234 | CA | ASN | B | 241 | -37.031 | 61.393 | 6.171 | 1.00 | 67.53 | 6 |
| | ATOM | 235 | CB | ASN | B | 241 | -38.240 | 60.846 | 6.915 | 1.00 | 67.98 | 6 |
| 10 | ATOM | 236 | CG | ASN | B | 241 | -37.966 | 59.479 | 7.544 | 1.00 | 70.19 | 6 |
| | ATOM | 237 | OD1 | ASN | B | 241 | -37.561 | 58.526 | 6.845 | 1.00 | 71.37 | 8 |
| | ATOM | 238 | ND2 | ASN | B | 241 | -38.205 | 59.370 | 8.836 | 1.00 | 71.48 | 7 |
| | ATOM | 239 | C | ASN | B | 241 | -37.496 | 62.532 | 5.255 | 1.00 | 66.62 | 6 |
| | ATOM | 240 | O | ASN | B | 241 | -38.504 | 62.395 | 4.578 | 1.00 | 64.76 | 8 |
| 15 | ATOM | 241 | N | LYS | B | 242 | -36.753 | 63.633 | 5.209 | 1.00 | 66.86 | 7 |
| | ATOM | 242 | CA | LYS | B | 242 | -37.096 | 64.772 | 4.362 | 1.00 | 67.46 | 6 |
| | ATOM | 243 | CB | LYS | B | 242 | -37.501 | 65.948 | 5.258 | 1.00 | 67.93 | 6 |
| | ATOM | 244 | CG | LYS | B | 242 | -38.746 | 65.684 | 6.076 | 1.00 | 71.52 | 6 |
| | ATOM | 245 | CD | LYS | B | 242 | -40.007 | 65.528 | 5.215 | 1.00 | 74.32 | 6 |
| 20 | ATOM | 246 | CE | LYS | B | 242 | -40.416 | 66.852 | 4.564 | 1.00 | 74.41 | 6 |
| | ATOM | 247 | NZ | LYS | B | 242 | -40.657 | 67.941 | 5.575 | 1.00 | 74.44 | 7 |
| | ATOM | 248 | C | LYS | B | 242 | -35.826 | 65.081 | 3.592 | 1.00 | 66.28 | 6 |
| | ATOM | 249 | O | LYS | B | 242 | -35.814 | 65.799 | 2.601 | 1.00 | 67.61 | 8 |
| | ATOM | 250 | N | ARG | B | 243 | -34.763 | 64.485 | 4.112 | 1.00 | 64.19 | 7 |
| 25 | ATOM | 251 | CA | ARG | B | 243 | -33.410 | 64.577 | 3.591 | 1.00 | 62.43 | 6 |
| | ATOM | 252 | CB | ARG | B | 243 | -32.599 | 63.547 | 4.390 | 1.00 | 60.12 | 6 |
| | ATOM | 253 | CG | ARG | B | 243 | -31.128 | 63.558 | 4.171 | 1.00 | 40.00 | 6 |
| | ATOM | 254 | CD | ARG | B | 243 | -30.335 | 62.888 | 5.319 | 1.00 | 40.00 | 6 |
| | ATOM | 255 | NE | ARG | B | 243 | -30.269 | 61.428 | 5.296 | 1.00 | 40.00 | 7 |
| 30 | ATOM | 256 | CZ | ARG | B | 243 | -29.384 | 60.724 | 6.009 | 1.00 | 40.00 | 6 |
| | ATOM | 257 | NH1 | ARG | B | 243 | -28.510 | 61.357 | 6.798 | 1.00 | 40.00 | 7 |
| | ATOM | 258 | NH2 | ARG | B | 243 | -29.355 | 59.401 | 5.908 | 1.00 | 40.00 | 7 |
| | ATOM | 259 | C | ARG | B | 243 | -33.408 | 64.252 | 2.100 | 1.00 | 62.97 | 6 |
| | ATOM | 260 | O | ARG | B | 243 | -33.690 | 63.122 | 1.722 | 1.00 | 63.96 | 8 |
| 35 | ATOM | 261 | N | LYS | B | 244 | -33.105 | 65.245 | 1.270 | 1.00 | 62.41 | 7 |
| | ATOM | 262 | CA | LYS | B | 244 | -33.054 | 65.053 | -0.179 | 1.00 | 61.57 | 6 |
| | ATOM | 263 | CB | LYS | B | 244 | -34.104 | 65.941 | -0.866 | 1.00 | 63.68 | 6 |
| | ATOM | 264 | CG | LYS | B | 244 | -35.527 | 65.731 | -0.337 | 1.00 | 71.29 | 6 |
| | ATOM | 265 | CD | LYS | B | 244 | -36.566 | 66.549 | -1.107 | 1.00 | 73.83 | 6 |
| 40 | ATOM | 266 | CE | LYS | B | 244 | -36.219 | 68.045 | -1.138 | 1.00 | 74.71 | 6 |
| | ATOM | 267 | NZ | LYS | B | 244 | -36.169 | 68.689 | 0.219 | 1.00 | 73.32 | 7 |
| | ATOM | 268 | C | LYS | B | 244 | -31.658 | 65.402 | -0.670 | 1.00 | 59.30 | 6 |
| | ATOM | 269 | O | LYS | B | 244 | -31.317 | 66.570 | -0.852 | 1.00 | 56.34 | 8 |
| | ATOM | 270 | N | PHE | B | 245 | -30.858 | 64.359 | -0.875 | 1.00 | 57.06 | 7 |
| 45 | ATOM | 271 | CA | PHE | B | 245 | -29.462 | 64.525 | -1.305 | 1.00 | 59.01 | 6 |
| | ATOM | 272 | CB | PHE | B | 245 | -28.786 | 63.179 | -1.478 | 1.00 | 59.62 | 6 |
| | ATOM | 273 | CG | PHE | B | 245 | -28.991 | 62.288 | -0.339 | 1.00 | 66.60 | 6 |
| | ATOM | 274 | CD1 | PHE | B | 245 | -30.200 | 61.669 | -0.172 | 1.00 | 67.17 | 6 |
| | ATOM | 275 | CD2 | PHE | B | 245 | -28.012 | 62.117 | 0.593 | 1.00 | 69.25 | 6 |
| 50 | ATOM | 276 | CE1 | PHE | B | 245 | -30.404 | 60.882 | 0.911 | 1.00 | 69.92 | 6 |
| | ATOM | 277 | CE2 | PHE | B | 245 | -28.229 | 61.329 | 1.669 | 1.00 | 70.50 | 6 |
| | ATOM | 278 | CZ | PHE | B | 245 | -29.418 | 60.714 | 1.830 | 1.00 | 70.89 | 6 |
| | ATOM | 279 | C | PHE | B | 245 | -29.301 | 65.282 | -2.592 | 1.00 | 60.68 | 6 |
| | ATOM | 280 | O | PHE | B | 245 | -29.859 | 64.911 | -3.619 | 1.00 | 62.37 | 8 |
| 55 | ATOM | 281 | N | LEU | B | 246 | -28.495 | 66.336 | -2.505 | 1.00 | 60.10 | 7 |
| | ATOM | 282 | CA | LEU | B | 246 | -28.201 | 67.199 | -3.631 | 1.00 | 59.44 | 6 |
| | ATOM | 283 | CB | LEU | B | 246 | -27.248 | 68.332 | -3.231 | 1.00 | 57.43 | 6 |
| | ATOM | 284 | CG | LEU | B | 246 | -27.118 | 69.474 | -4.207 | 1.00 | 54.41 | 6 |

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|----|------|-----|-----|-----|---|-----|---------|--------|---------|------|-------|---|
| 5 | ATOM | 285 | CD1 | LEU | B | 246 | -28.481 | 70.137 | -4.349 | 1.00 | 52.43 | 6 |
| | ATOM | 286 | CD2 | LEU | B | 246 | -26.112 | 70.470 | -3.719 | 1.00 | 51.69 | 6 |
| | ATOM | 287 | C | LEU | B | 246 | -27.585 | 66.379 | -4.740 | 1.00 | 62.05 | 6 |
| | ATOM | 288 | O | LEU | B | 246 | -26.789 | 65.446 | -4.486 | 1.00 | 59.85 | 8 |
| | ATOM | 289 | N | PRO | B | 247 | -27.930 | 66.693 | -5.984 | 1.00 | 63.33 | 7 |
| 10 | ATOM | 290 | CD | PRO | B | 247 | -28.839 | 67.781 | -6.363 | 1.00 | 64.44 | 6 |
| | ATOM | 291 | CA | PRO | B | 247 | -27.391 | 65.958 | -7.130 | 1.00 | 63.56 | 6 |
| | ATOM | 292 | CB | PRO | B | 247 | -27.976 | 66.675 | -8.340 | 1.00 | 64.42 | 6 |
| | ATOM | 293 | CG | PRO | B | 247 | -28.873 | 67.714 | -7.841 | 1.00 | 64.90 | 6 |
| | ATOM | 294 | C | PRO | B | 247 | -25.866 | 65.947 | -7.143 | 1.00 | 61.94 | 6 |
| 15 | ATOM | 295 | O | PRO | B | 247 | -25.223 | 66.944 | -6.856 | 1.00 | 61.60 | 8 |
| | ATOM | 296 | N | GLU | B | 248 | -25.333 | 64.771 | -7.478 | 1.00 | 61.33 | 7 |
| | ATOM | 297 | CA | GLU | B | 248 | -23.896 | 64.516 | -7.590 | 1.00 | 63.50 | 6 |
| | ATOM | 298 | CB | GLU | B | 248 | -23.630 | 63.154 | -8.248 | 1.00 | 66.94 | 6 |
| | ATOM | 299 | CG | GLU | B | 248 | -22.168 | 62.953 | -8.713 | 1.00 | 68.70 | 6 |
| 20 | ATOM | 300 | CD | GLU | B | 248 | -21.898 | 61.745 | -9.580 | 1.00 | 40.00 | 6 |
| | ATOM | 301 | OE1 | GLU | B | 248 | -22.863 | 61.007 | -10.035 | 1.00 | 40.00 | 8 |
| | ATOM | 302 | OE2 | GLU | B | 248 | -20.709 | 61.460 | -9.838 | 1.00 | 40.00 | 8 |
| | ATOM | 303 | C | GLU | B | 248 | -23.158 | 65.571 | -8.415 | 1.00 | 64.19 | 6 |
| | ATOM | 304 | O | GLU | B | 248 | -22.056 | 65.975 | -8.066 | 1.00 | 65.56 | 8 |
| 25 | ATOM | 305 | N | ASP | B | 249 | -23.796 | 66.019 | -9.498 | 1.00 | 64.36 | 7 |
| | ATOM | 306 | CA | ASP | B | 249 | -23.254 | 66.994 | -10.436 | 1.00 | 63.33 | 6 |
| | ATOM | 307 | CB | ASP | B | 249 | -24.122 | 67.031 | -11.698 | 1.00 | 62.97 | 6 |
| | ATOM | 308 | CG | ASP | B | 249 | -25.437 | 67.715 | -11.489 | 1.00 | 64.63 | 6 |
| | ATOM | 309 | OD1 | ASP | B | 249 | -26.235 | 67.285 | -10.629 | 1.00 | 64.84 | 8 |
| 30 | ATOM | 310 | OD2 | ASP | B | 249 | -25.726 | 68.718 | -12.189 | 1.00 | 66.52 | 8 |
| | ATOM | 311 | C | ASP | B | 249 | -23.068 | 68.413 | -9.960 | 1.00 | 64.31 | 6 |
| | ATOM | 312 | O | ASP | B | 249 | -22.117 | 69.084 | -10.355 | 1.00 | 64.73 | 8 |
| | ATOM | 313 | N | ILE | B | 250 | -23.987 | 68.892 | -9.136 | 1.00 | 63.09 | 7 |
| | ATOM | 314 | CA | ILE | B | 250 | -23.921 | 70.281 | -8.660 | 1.00 | 64.39 | 6 |
| 35 | ATOM | 315 | CB | ILE | B | 250 | -25.124 | 70.575 | -7.798 | 1.00 | 65.79 | 6 |
| | ATOM | 316 | CG2 | ILE | B | 250 | -25.559 | 72.041 | -7.858 | 1.00 | 64.78 | 6 |
| | ATOM | 317 | CG1 | ILE | B | 250 | -26.348 | 69.752 | -8.206 | 1.00 | 65.28 | 6 |
| | ATOM | 318 | CD1 | ILE | B | 250 | -27.671 | 70.444 | -7.887 | 1.00 | 65.08 | 6 |
| | ATOM | 319 | C | ILE | B | 250 | -22.815 | 70.488 | -7.714 | 1.00 | 65.21 | 6 |
| 40 | ATOM | 320 | O | ILE | B | 250 | -22.754 | 69.847 | -6.656 | 1.00 | 64.05 | 8 |
| | ATOM | 321 | N | GLY | B | 251 | -22.024 | 71.392 | -8.103 | 1.00 | 65.48 | 7 |
| | ATOM | 322 | CA | GLY | B | 251 | -20.873 | 71.721 | -7.342 | 1.00 | 67.32 | 6 |
| | ATOM | 323 | C | GLY | B | 251 | -19.808 | 70.806 | -7.800 | 1.00 | 68.52 | 6 |
| | ATOM | 324 | O | GLY | B | 251 | -19.791 | 70.548 | -9.025 | 1.00 | 65.49 | 8 |
| 45 | ATOM | 325 | N | GLN | B | 252 | -19.074 | 70.440 | -6.799 | 1.00 | 72.26 | 7 |
| | ATOM | 326 | CA | GLN | B | 252 | -17.949 | 69.540 | -6.883 | 1.00 | 74.10 | 6 |
| | ATOM | 327 | CB | GLN | B | 252 | -18.460 | 68.098 | -6.723 | 1.00 | 75.82 | 6 |
| | ATOM | 328 | CG | GLN | B | 252 | -17.367 | 67.088 | -6.356 | 1.00 | 77.81 | 6 |
| | ATOM | 329 | CD | GLN | B | 252 | -17.924 | 65.759 | -5.824 | 1.00 | 79.38 | 6 |
| 50 | ATOM | 330 | OE1 | GLN | B | 252 | -18.615 | 65.042 | -6.549 | 1.00 | 80.55 | 8 |
| | ATOM | 331 | NE2 | GLN | B | 252 | -17.661 | 65.380 | -4.586 | 1.00 | 78.12 | 7 |
| | ATOM | 332 | C | GLN | B | 252 | -17.258 | 69.727 | -8.258 | 1.00 | 77.17 | 6 |
| | ATOM | 333 | O | GLN | B | 252 | -17.977 | 70.009 | -9.227 | 1.00 | 76.50 | 8 |
| | ATOM | 334 | N | ALA | B | 253 | -15.718 | 69.795 | -8.279 | 1.00 | 80.78 | 7 |
| 55 | ATOM | 335 | CA | ALA | B | 253 | -14.615 | 70.766 | -8.544 | 1.00 | 83.70 | 6 |
| | ATOM | 336 | CB | ALA | B | 253 | -13.794 | 70.914 | -7.255 | 1.00 | 83.23 | 6 |
| | ATOM | 337 | C | ALA | B | 253 | -13.605 | 70.732 | -9.731 | 1.00 | 85.59 | 6 |
| | ATOM | 338 | O | ALA | B | 253 | -13.186 | 69.691 | -10.171 | 1.00 | 85.69 | 8 |

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|----|------|-----|-----|-----------|---------|--------|---------|------|-------|---|
| 5 | ATOM | 339 | N | PRO B 254 | -13.223 | 71.944 | -11.715 | 1.00 | 39.05 | 7 |
| | ATOM | 340 | CD | PRO B 254 | -13.798 | 73.217 | -9.752 | 1.00 | 33.97 | 6 |
| | ATOM | 341 | CA | PRO B 254 | -12.266 | 72.177 | -11.351 | 1.00 | 35.89 | 6 |
| | ATOM | 342 | CB | PRO B 254 | -12.275 | 73.710 | -11.596 | 1.00 | 33.94 | 6 |
| | ATOM | 343 | CG | PRO B 254 | -13.222 | 74.277 | -10.688 | 1.00 | 33.31 | 6 |
| 10 | ATOM | 344 | C | PRO B 254 | -10.827 | 71.665 | -11.121 | 1.00 | 37.75 | 6 |
| | ATOM | 345 | O | PRO B 254 | -10.379 | 71.426 | -10.009 | 1.00 | 38.78 | 8 |
| | TER | | | | | | | | | |
| | ATOM | 1 | N | GLY B 261 | -8.238 | 79.356 | -2.979 | 1.00 | 40.00 | 7 |
| | ATOM | 2 | CA | GLY B 261 | -9.314 | 78.411 | -3.005 | 1.00 | 40.00 | 6 |
| 15 | ATOM | 3 | C | GLY B 261 | -10.206 | 78.717 | -4.355 | 1.00 | 40.00 | 6 |
| | ATOM | 4 | O | GLY B 261 | -11.372 | 79.141 | -4.256 | 1.00 | 40.00 | 8 |
| | ATOM | 5 | N | GLY B 262 | -9.565 | 78.527 | -5.597 | 1.00 | 40.00 | 7 |
| | ATOM | 6 | CA | GLY B 262 | -10.136 | 78.609 | -7.087 | 1.00 | 40.00 | 6 |
| | ATOM | 7 | C | GLY B 262 | -10.849 | 79.966 | -7.577 | 1.00 | 40.00 | 6 |
| 20 | ATOM | 8 | O | GLY B 262 | -10.200 | 81.044 | -7.543 | 1.00 | 40.00 | 8 |
| | ATOM | 9 | N | LYS B 263 | -12.086 | 79.687 | -8.124 | 1.00 | 61.71 | 7 |
| | ATOM | 10 | CA | LYS B 263 | -13.323 | 80.536 | -8.428 | 1.00 | 64.36 | 6 |
| | ATOM | 11 | C | LYS B 263 | -14.367 | 79.750 | -7.614 | 1.00 | 63.41 | 6 |
| | ATOM | 12 | O | LYS B 263 | -14.102 | 78.579 | -7.280 | 1.00 | 61.93 | 8 |
| 25 | ATOM | 13 | CB | LYS B 263 | -13.901 | 80.405 | -9.876 | 1.00 | 63.50 | 6 |
| | ATOM | 14 | CG | LYS B 263 | -13.487 | 81.474 | -10.881 | 1.00 | 20.00 | 6 |
| | ATOM | 15 | CD | LYS B 263 | -14.016 | 82.897 | -10.612 | 1.00 | 20.00 | 6 |
| | ATOM | 16 | CE | LYS B 263 | -13.641 | 83.874 | -11.742 | 1.00 | 20.00 | 6 |
| | ATOM | 17 | NZ | LYS B 263 | -13.680 | 85.287 | -11.341 | 1.00 | 20.00 | 7 |
| 30 | ATOM | 18 | N | VAL B 264 | -15.489 | 80.335 | -7.307 | 1.00 | 61.15 | 7 |
| | ATOM | 19 | CA | VAL B 264 | -16.616 | 79.632 | -6.619 | 1.00 | 59.46 | 6 |
| | ATOM | 20 | CB | VAL B 264 | -17.574 | 80.703 | -6.099 | 1.00 | 59.03 | 6 |
| | ATOM | 21 | CG1 | VAL B 264 | -18.479 | 80.215 | -4.979 | 1.00 | 53.79 | 6 |
| | ATOM | 22 | CG2 | VAL B 264 | -16.847 | 81.938 | -5.562 | 1.00 | 55.32 | 6 |
| 35 | ATOM | 23 | C | VAL B 264 | -17.330 | 78.824 | -7.700 | 1.00 | 60.96 | 6 |
| | ATOM | 24 | O | VAL B 264 | -16.940 | 78.873 | -8.873 | 1.00 | 62.13 | 8 |
| | ATOM | 25 | N | ASP B 265 | -18.378 | 78.098 | -7.340 | 1.00 | 62.59 | 7 |
| | ATOM | 26 | CA | ASP B 265 | -19.175 | 77.339 | -8.312 | 1.00 | 64.95 | 6 |
| | ATOM | 27 | CB | ASP B 265 | -18.796 | 75.851 | -8.270 | 1.00 | 64.32 | 6 |
| 40 | ATOM | 28 | CG | ASP B 265 | -19.928 | 75.022 | -8.584 | 1.00 | 67.70 | 6 |
| | ATOM | 29 | OD1 | ASP B 265 | -20.856 | 75.062 | -9.295 | 1.00 | 72.59 | 8 |
| | ATOM | 30 | OD2 | ASP B 265 | -20.370 | 73.959 | -8.310 | 1.00 | 68.84 | 8 |
| | ATOM | 31 | C | ASP B 265 | -20.658 | 77.614 | -8.016 | 1.00 | 65.64 | 6 |
| | ATOM | 32 | O | ASP B 265 | -21.342 | 76.895 | -7.313 | 1.00 | 68.81 | 8 |
| 45 | ATOM | 33 | N | LEU B 266 | -21.066 | 78.737 | -8.588 | 1.00 | 65.12 | 7 |
| | ATOM | 34 | CA | LEU B 266 | -22.385 | 79.330 | -8.499 | 1.00 | 63.40 | 6 |
| | ATOM | 35 | CB | LEU B 266 | -22.429 | 80.448 | -9.542 | 1.00 | 67.34 | 6 |
| | ATOM | 36 | CG | LEU B 266 | -21.295 | 81.459 | -9.399 | 1.00 | 69.35 | 6 |
| | ATOM | 37 | CD1 | LEU B 266 | -20.983 | 82.127 | -10.712 | 1.00 | 68.24 | 6 |
| 50 | ATOM | 38 | CD2 | LEU B 266 | -21.663 | 82.461 | -8.344 | 1.00 | 70.47 | 6 |
| | ATOM | 39 | C | LEU B 266 | -23.673 | 78.507 | -8.602 | 1.00 | 59.67 | 6 |
| | ATOM | 40 | O | LEU B 266 | -24.684 | 78.890 | -7.988 | 1.00 | 53.35 | 8 |
| | ATOM | 41 | N | GLU B 267 | -23.677 | 77.416 | -9.371 | 1.00 | 58.01 | 7 |
| | ATOM | 42 | CA | GLU B 267 | -24.901 | 76.640 | -9.449 | 1.00 | 58.34 | 6 |
| 55 | ATOM | 43 | CB | GLU B 267 | -24.752 | 75.410 | -10.368 | 1.00 | 59.21 | 6 |
| | ATOM | 44 | CG | GLU B 267 | -25.979 | 74.464 | -10.268 | 1.00 | 62.89 | 6 |
| | ATOM | 45 | CD | GLU B 267 | -26.048 | 73.419 | -11.328 | 1.00 | 67.66 | 6 |
| | ATOM | 46 | OE1 | GLU B 267 | -25.076 | 72.645 | -11.512 | 1.00 | 69.95 | 8 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------------------|-----------------|------------------|---|
| 5 | ATOM | 47 | OE2 | GLU | B | 267 | -27.098 | 73.328 | -12.068 | 4.00 | 69.40 | 8 |
| | ATOM | 48 | C | GLU | B | 267 | -25.200 | 76.184 | -8.032 | 1.00 | 57.67 | 6 |
| | ATOM | 49 | O | GLU | B | 267 | -26.354 | 76.009 | -7.643 | 1.00 | 58.34 | 8 |
| | ATOM | 50 | N | ALA | B | 268 | -24.114 | 75.996 | -7.285 | 1.00 | 53.43 | 7 |
| | ATOM | 51 | CA | ALA | B | 268 | -24.151 | 75.560 | -5.905 | 1.00 | 49.00 | 6 |
| 10 | ATOM | 52 | CB | ALA | B | 268 | -22.816 | 74.956 | -5.526 | 1.00 | 45.72 | 6 |
| | ATOM | 53 | C | ALA | B | 268 | -24.421 | 76.775 | -5.056 | 1.00 | 45.76 | 6 |
| | ATOM | 54 | O | ALA | B | 268 | -25.419 | 76.823 | -4.351 | 1.00 | 41.50 | 8 |
| | ATOM | 55 | N | PHE | B | 269 | -23.533 | 77.766 | -5.142 | 1.00 | 41.43 | 7 |
| | ATOM | 56 | CA | PHE | B | 269 | -23.688 | 78.989 | -4.358 | 1.00 | 43.96 | 6 |
| 15 | ATOM | 57 | CB | PHE | B | 269 | -22.903 | 80.150 | -4.971 | 1.00 | 40.10 | 6 |
| | ATOM | 58 | CG | PHE | B | 269 | -23.057 | 81.458 | -4.224 | 1.00 | 40.44 | 6 |
| | ATOM | 59 | CD1 | PHE | B | 269 | -22.284 | 81.727 | -3.105 | 1.00 | 38.98 | 6 |
| | ATOM | 60 | CD2 | PHE | B | 269 | -24.033 | 82.372 | -4.603 | 1.00 | 37.15 | 6 |
| | ATOM | 61 | CE1 | PHE | B | 269 | -22.472 | 82.921 | -2.388 | 1.00 | 32.12 | 6 |
| 20 | ATOM | 62 | CE2 | PHE | B | 269 | -24.228 | 83.567 | -3.890 | 1.00 | 38.41 | 6 |
| | ATOM | 63 | CZ | PHE | B | 269 | -23.457 | 83.838 | -2.780 | 1.00 | 40.55 | 6 |
| | ATOM | 64 | C | PHE | B | 269 | -25.154 | 79.374 | -4.320 | 1.00 | 49.76 | 6 |
| | ATOM | 65 | O | PHE | B | 269 | -25.645 | 79.905 | -3.336 | 1.00 | 52.15 | 8 |
| | ATOM | 66 | N | SER | B | 270 | -25.840 | 79.112 | -5.426 | 1.00 | 53.15 | 7 |
| 25 | ATOM | 67 | CA | SER | B | 270 | -27.253 | 79.431 | -5.520 | 1.00 | 52.29 | 6 |
| | ATOM | 68 | CB | SER | B | 270 | -27.742 | 79.274 | -6.948 | 1.00 | 51.85 | 6 |
| | ATOM | 69 | OG | SER | B | 270 | -29.118 | 79.606 | -7.048 | 1.00 | 53.42 | 8 |
| | ATOM | 70 | C | SER | B | 270 | -28.012 | 78.486 | -4.630 | 1.00 | 49.38 | 6 |
| | ATOM | 71 | O | SER | B | 270 | -28.438 | 78.864 | -3.548 | 1.00 | 48.74 | 8 |
| 30 | ATOM | 72 | N | HIS | B | 271 | -28.185 | 77.253 | -5.115 | 1.00 | 50.15 | 7 |
| | ATOM | 73 | CA | HIS | B | 271 | -28.904 | 76.203 | -4.382 | 1.00 | 51.67 | 6 |
| | ATOM | 74 | CB | HIS | B | 271 | -28.409 | 74.812 | -4.782 | 1.00 | 58.52 | 6 |
| | ATOM | 75 | CG | HIS | B | 271 | -29.096 | 74.248 | -5.976 | 1.00 | 68.97 | 6 |
| | ATOM | 76 | CD2 | HIS | B | 271 | -29.987 | 73.233 | -6.102 | 1.00 | 70.88 | 6 |
| 35 | ATOM | 77 | ND1 | HIS | B | 271 | -28.943 | 74.770 | -7.270 | 1.00 | 71.98 | 7 |
| | ATOM | 78 | CE1 | HIS | B | 271 | -29.716 | 74.080 | -8.100 | 1.00 | 73.91 | 6 |
| | ATOM | 79 | NE2 | HIS | B | 271 | -30.354 | 73.149 | -7.419 | 1.00 | 73.59 | 7 |
| | ATOM | 80 | C | HIS | B | 271 | -28.785 | 76.347 | -2.886 | 1.00 | 48.33 | 6 |
| | ATOM | 81 | O | HIS | B | 271 | -29.641 | 75.874 | -2.156 | 1.00 | 48.39 | 8 |
| 40 | ATOM | 82 | N | PHE | B | 272 | -27.702 | 76.992 | -2.444 | 1.00 | 41.34 | 7 |
| | ATOM | 83 | CA | PHE | B | 272 | -27.440 | 77.224 | -1.033 | 1.00 | 39.44 | 6 |
| | ATOM | 84 | CB | PHE | B | 272 | -25.936 | 77.302 | -0.801 | 1.00 | 36.67 | 6 |
| | ATOM | 85 | CG | PHE | B | 272 | -25.241 | 75.945 | -0.861 | 1.00 | 33.39 | 6 |
| | ATOM | 86 | CD1 | PHE | B | 272 | -23.856 | 75.857 | -0.976 | 1.00 | 33.14 | 6 |
| 45 | ATOM | 87 | CD2 | PHE | B | 272 | -25.973 | 74.767 | -0.732 | 1.00 | 38.28 | 6 |
| | ATOM | 88 | CE1 | PHE | B | 272 | -23.200 | 74.606 | -0.989 | 1.00 | 38.26 | 6 |
| | ATOM | 89 | CE2 | PHE | B | 272 | -25.321 | 73.518 | -0.743 | 1.00 | 43.28 | 6 |
| | ATOM | 90 | CZ | PHE | B | 272 | -23.937 | 73.441 | -0.856 | 1.00 | 39.74 | 6 |
| | ATOM | 91 | C | PHE | B | 272 | -28.144 | 78.472 | -0.477 | 1.00 | 40.75 | 6 |
| 50 | ATOM | 92 | O | PHE | B | 272 | -28.803 | 78.393 | 0.558 | 1.00 | 35.51 | 8 |
| | ATOM | 93 | N | THR | B | 273 | -28.027 | 79.621 | -1.144 | 1.00 | 41.64 | 7 |
| | ATOM | 94 | CA | THR | B | 273 | -28.658 | 80.850 | -0.652 | 1.00 | 45.97 | 6 |
| | ATOM | 95 | CB | THR | B | 273 | -28.023 | 82.105 | -1.283 | 1.00 | 51.52 | 6 |
| | ATOM | 96 | OG1 | THR | B | 273 | -28.292 | 82.151 | -2.688 | 1.00 | 45.74 | 8 |
| 55 | ATOM | 97 | CG2 | THR | B | 273 | -26.511 | 82.123 | -1.048 | 1.00 | 49.73 | 6 |
| | ATOM | 98 | C | THR | B | 273 | -30.142 | 80.859 | -0.971 | 1.00 | 46.23 | 6 |
| | ATOM | 99 | O | THR | B | 273 | -30.862 | 81.751 | -0.535 | 1.00 | 41.21 | 8 |
| | ATOM | 100 | N | LYS | B | 274 | -30.583 | 79.876 | -1.758 | 1.00 | 46.21 | 7 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 101 | CA | LYS | B | 274 | -31.983 | 79.774 | -2.147 | 1.00 | 54.53 | 6 |
| | ATOM | 102 | CB | LYS | B | 274 | -32.133 | 78.724 | -3.232 | 1.00 | 54.36 | 6 |
| | ATOM | 103 | C | LYS | B | 274 | -32.819 | 79.396 | -0.931 | 1.00 | 56.88 | 6 |
| | ATOM | 104 | O | LYS | B | 274 | -34.025 | 79.624 | -0.906 | 1.00 | 57.98 | 8 |
| | ATOM | 105 | N | ILE | B | 275 | -32.151 | 78.820 | 0.076 | 1.00 | 56.48 | 7 |
| 10 | ATOM | 106 | CA | ILE | B | 275 | -32.791 | 78.381 | 1.332 | 1.00 | 52.64 | 6 |
| | ATOM | 107 | CB | ILE | B | 275 | -32.638 | 76.863 | 1.519 | 1.00 | 49.15 | 6 |
| | ATOM | 108 | CG2 | ILE | B | 275 | -33.505 | 76.105 | 0.529 | 1.00 | 47.42 | 6 |
| | ATOM | 109 | CG1 | ILE | B | 275 | -31.188 | 76.441 | 1.343 | 1.00 | 45.31 | 6 |
| | ATOM | 110 | CD1 | ILE | B | 275 | -30.990 | 74.952 | 1.391 | 1.00 | 37.22 | 6 |
| 15 | ATOM | 111 | C | ILE | B | 275 | -32.241 | 79.086 | 2.574 | 1.00 | 51.78 | 6 |
| | ATOM | 112 | O | ILE | B | 275 | -32.858 | 79.049 | 3.622 | 1.00 | 49.80 | 8 |
| | ATOM | 113 | N | ILE | B | 276 | -31.071 | 79.709 | 2.435 | 1.00 | 51.76 | 7 |
| | ATOM | 114 | CA | ILE | B | 276 | -30.410 | 80.409 | 3.533 | 1.00 | 52.58 | 6 |
| | ATOM | 115 | CB | ILE | B | 276 | -29.145 | 81.110 | 3.042 | 1.00 | 55.04 | 6 |
| 20 | ATOM | 116 | CG2 | ILE | B | 276 | -29.486 | 82.172 | 2.017 | 1.00 | 53.28 | 6 |
| | ATOM | 117 | CG1 | ILE | B | 276 | -28.396 | 81.786 | 4.203 | 1.00 | 57.31 | 6 |
| | ATOM | 118 | CD1 | ILE | B | 276 | -27.862 | 80.854 | 5.231 | 1.00 | 60.32 | 6 |
| | ATOM | 119 | C | ILE | B | 276 | -31.282 | 81.461 | 4.237 | 1.00 | 50.70 | 6 |
| | ATOM | 120 | O | ILE | B | 276 | -31.015 | 81.817 | 5.385 | 1.00 | 55.55 | 8 |
| 25 | ATOM | 121 | N | THR | B | 277 | -32.322 | 81.953 | 3.568 | 1.00 | 47.33 | 7 |
| | ATOM | 122 | CA | THR | B | 277 | -33.174 | 82.968 | 4.141 | 1.00 | 42.59 | 6 |
| | ATOM | 123 | CB | THR | B | 277 | -34.042 | 83.632 | 3.048 | 1.00 | 44.97 | 6 |
| | ATOM | 124 | OG1 | THR | B | 277 | -33.202 | 84.145 | 2.001 | 1.00 | 46.38 | 8 |
| | ATOM | 125 | CG2 | THR | B | 277 | -34.856 | 84.781 | 3.653 | 1.00 | 37.17 | 6 |
| 30 | ATOM | 126 | C | THR | B | 277 | -34.069 | 82.447 | 5.267 | 1.00 | 39.84 | 6 |
| | ATOM | 127 | O | THR | B | 277 | -34.083 | 83.026 | 6.375 | 1.00 | 40.55 | 8 |
| | ATOM | 128 | N | PRO | B | 278 | -34.832 | 81.385 | 5.017 | 1.00 | 38.20 | 7 |
| | ATOM | 129 | CD | PRO | B | 278 | -34.925 | 80.666 | 3.747 | 1.00 | 36.34 | 6 |
| | ATOM | 130 | CA | PRO | B | 278 | -35.711 | 80.834 | 6.059 | 1.00 | 36.63 | 6 |
| 35 | ATOM | 131 | CB | PRO | B | 278 | -36.475 | 79.715 | 5.357 | 1.00 | 32.95 | 6 |
| | ATOM | 132 | CG | PRO | B | 278 | -35.833 | 79.516 | 4.056 | 1.00 | 35.75 | 6 |
| | ATOM | 133 | C | PRO | B | 278 | -34.892 | 80.324 | 7.220 | 1.00 | 38.60 | 6 |
| | ATOM | 134 | O | PRO | B | 278 | -35.372 | 80.157 | 8.331 | 1.00 | 37.67 | 8 |
| | ATOM | 135 | N | ALA | B | 279 | -33.636 | 80.040 | 6.927 | 1.00 | 37.05 | 7 |
| 40 | ATOM | 136 | CA | ALA | B | 279 | -32.696 | 79.525 | 7.903 | 1.00 | 33.18 | 6 |
| | ATOM | 137 | CB | ALA | B | 279 | -31.391 | 79.195 | 7.205 | 1.00 | 30.56 | 6 |
| | ATOM | 138 | C | ALA | B | 279 | -32.447 | 80.536 | 8.991 | 1.00 | 33.47 | 6 |
| | ATOM | 139 | O | ALA | B | 279 | -32.623 | 80.238 | 10.158 | 1.00 | 33.74 | 8 |
| | ATOM | 140 | N | ILE | B | 280 | -32.010 | 81.728 | 8.577 | 1.00 | 29.96 | 7 |
| 45 | ATOM | 141 | CA | ILE | B | 280 | -31.728 | 82.809 | 9.501 | 1.00 | 25.94 | 6 |
| | ATOM | 142 | CB | ILE | B | 280 | -31.190 | 84.040 | 8.754 | 1.00 | 26.95 | 6 |
| | ATOM | 143 | CG2 | ILE | B | 280 | -30.881 | 85.149 | 9.715 | 1.00 | 15.40 | 6 |
| | ATOM | 144 | CG1 | ILE | B | 280 | -29.904 | 83.696 | 8.007 | 1.00 | 26.73 | 6 |
| | ATOM | 145 | CD1 | ILE | B | 280 | -29.255 | 84.878 | 7.362 | 1.00 | 34.31 | 6 |
| 50 | ATOM | 146 | C | ILE | B | 280 | -32.964 | 83.172 | 10.310 | 1.00 | 31.39 | 6 |
| | ATOM | 147 | O | ILE | B | 280 | -32.882 | 83.378 | 11.522 | 1.00 | 35.69 | 8 |
| | ATOM | 148 | N | THR | B | 281 | -34.113 | 83.233 | 9.647 | 1.00 | 30.90 | 7 |
| | ATOM | 149 | CA | THR | B | 281 | -35.361 | 83.586 | 10.328 | 1.00 | 33.49 | 6 |
| | ATOM | 150 | CB | THR | B | 281 | -36.598 | 83.396 | 9.419 | 1.00 | 37.18 | 6 |
| 55 | ATOM | 151 | OG1 | THR | B | 281 | -36.703 | 82.034 | 9.005 | 1.00 | 46.48 | 8 |
| | ATOM | 152 | CG2 | THR | B | 281 | -36.525 | 84.289 | 8.198 | 1.00 | 32.85 | 6 |
| | ATOM | 153 | C | THR | B | 281 | -35.523 | 82.706 | 11.556 | 1.00 | 29.94 | 6 |
| | ATOM | 154 | O | THR | B | 281 | -35.855 | 83.186 | 12.634 | 1.00 | 25.55 | 8 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 155 | N | ARG | B | 282 | -35.296 | 81.405 | 11.378 | 1.00 | 32.70 | 7 |
| | ATOM | 156 | CA | ARG | B | 282 | -35.439 | 80.449 | 12.475 | 1.00 | 34.27 | 6 |
| | ATOM | 157 | CB | ARG | B | 282 | -34.999 | 79.060 | 12.020 | 1.00 | 33.78 | 6 |
| | ATOM | 158 | CG | ARG | B | 282 | -35.986 | 77.944 | 12.280 | 1.00 | 45.15 | 6 |
| | ATOM | 159 | CD | ARG | B | 282 | -36.701 | 77.514 | 11.015 | 1.00 | 58.24 | 6 |
| 10 | ATOM | 160 | NE | ARG | B | 282 | -35.771 | 77.153 | 9.969 | 1.00 | 68.41 | 7 |
| | ATOM | 161 | CZ | ARG | B | 282 | -34.862 | 76.200 | 10.098 | 1.00 | 72.31 | 6 |
| | ATOM | 162 | NH1 | ARG | B | 282 | -34.779 | 75.502 | 11.232 | 1.00 | 77.89 | 7 |
| | ATOM | 163 | NH2 | ARG | B | 282 | -34.022 | 75.963 | 9.096 | 1.00 | 69.25 | 7 |
| | ATOM | 164 | C | ARG | B | 282 | -34.556 | 80.919 | 13.622 | 1.00 | 34.81 | 6 |
| 15 | ATOM | 165 | O | ARG | B | 282 | -35.008 | 81.034 | 14.753 | 1.00 | 36.03 | 8 |
| | ATOM | 166 | N | VAL | B | 283 | -33.288 | 81.183 | 13.289 | 1.00 | 31.71 | 7 |
| | ATOM | 167 | CA | VAL | B | 283 | -32.304 | 81.667 | 14.249 | 1.00 | 30.16 | 6 |
| | ATOM | 168 | CB | VAL | B | 283 | -30.993 | 82.029 | 13.559 | 1.00 | 29.00 | 6 |
| | ATOM | 169 | CG1 | VAL | B | 283 | -30.015 | 82.617 | 14.557 | 1.00 | 28.64 | 6 |
| 20 | ATOM | 170 | CG2 | VAL | B | 283 | -30.385 | 80.816 | 12.915 | 1.00 | 28.28 | 6 |
| | ATOM | 171 | C | VAL | B | 283 | -32.848 | 82.884 | 14.994 | 1.00 | 32.50 | 6 |
| | ATOM | 172 | O | VAL | B | 283 | -32.619 | 83.057 | 16.185 | 1.00 | 33.48 | 8 |
| | ATOM | 173 | N | VAL | B | 284 | -33.573 | 83.728 | 14.265 | 1.00 | 30.96 | 7 |
| | ATOM | 174 | CA | VAL | B | 284 | -34.177 | 84.925 | 14.844 | 1.00 | 29.14 | 6 |
| 25 | ATOM | 175 | CB | VAL | B | 284 | -34.672 | 85.892 | 13.751 | 1.00 | 31.27 | 6 |
| | ATOM | 176 | CG1 | VAL | B | 284 | -35.278 | 87.129 | 14.371 | 1.00 | 24.21 | 6 |
| | ATOM | 177 | CG2 | VAL | B | 284 | -33.554 | 86.270 | 12.812 | 1.00 | 30.51 | 6 |
| | ATOM | 178 | C | VAL | B | 284 | -35.336 | 84.498 | 15.747 | 1.00 | 28.89 | 6 |
| | ATOM | 179 | O | VAL | B | 284 | -35.491 | 84.994 | 16.860 | 1.00 | 27.29 | 8 |
| 30 | ATOM | 180 | N | ASP | B | 285 | -36.143 | 83.564 | 15.250 | 1.00 | 28.76 | 7 |
| | ATOM | 181 | CA | ASP | B | 285 | -37.299 | 83.057 | 15.983 | 1.00 | 35.32 | 6 |
| | ATOM | 182 | CB | ASP | B | 285 | -38.129 | 82.098 | 15.111 | 1.00 | 33.29 | 6 |
| | ATOM | 183 | CG | ASP | B | 285 | -38.881 | 82.795 | 14.013 | 1.00 | 38.15 | 6 |
| | ATOM | 184 | OD1 | ASP | B | 285 | -39.660 | 83.729 | 14.305 | 1.00 | 34.70 | 8 |
| 35 | ATOM | 185 | OD2 | ASP | B | 285 | -38.741 | 82.406 | 12.821 | 1.00 | 34.43 | 8 |
| | ATOM | 186 | C | ASP | B | 285 | -36.863 | 82.339 | 17.257 | 1.00 | 36.70 | 6 |
| | ATOM | 187 | O | ASP | B | 285 | -37.606 | 82.304 | 18.237 | 1.00 | 37.96 | 8 |
| | ATOM | 188 | N | PHE | B | 286 | -35.663 | 81.755 | 17.235 | 1.00 | 35.96 | 7 |
| | ATOM | 189 | CA | PHE | B | 286 | -35.134 | 81.053 | 18.401 | 1.00 | 37.10 | 6 |
| 40 | ATOM | 190 | CB | PHE | B | 286 | -33.870 | 80.262 | 18.052 | 1.00 | 37.97 | 6 |
| | ATOM | 191 | CG | PHE | B | 286 | -33.079 | 79.818 | 19.258 | 1.00 | 36.50 | 6 |
| | ATOM | 192 | CD1 | PHE | B | 286 | -33.704 | 79.168 | 20.294 | 1.00 | 36.75 | 6 |
| | ATOM | 193 | CD2 | PHE | B | 286 | -31.721 | 80.063 | 19.343 | 1.00 | 33.83 | 6 |
| | ATOM | 194 | CE1 | PHE | B | 286 | -32.987 | 78.769 | 21.401 | 1.00 | 39.55 | 6 |
| 45 | ATOM | 195 | CE2 | PHE | B | 286 | -30.997 | 79.662 | 20.456 | 1.00 | 38.08 | 6 |
| | ATOM | 196 | CZ | PHE | B | 286 | -31.632 | 79.013 | 21.486 | 1.00 | 34.44 | 6 |
| | ATOM | 197 | C | PHE | B | 286 | -34.808 | 82.023 | 19.504 | 1.00 | 36.83 | 6 |
| | ATOM | 198 | O | PHE | B | 286 | -35.246 | 81.845 | 20.631 | 1.00 | 35.61 | 8 |
| | ATOM | 199 | N | ALA | B | 287 | -34.005 | 83.027 | 19.169 | 1.00 | 37.33 | 7 |
| 50 | ATOM | 200 | CA | ALA | B | 287 | -33.599 | 84.035 | 20.132 | 1.00 | 36.34 | 6 |
| | ATOM | 201 | CB | ALA | B | 287 | -32.644 | 85.008 | 19.469 | 1.00 | 36.40 | 6 |
| | ATOM | 202 | C | ALA | B | 287 | -34.831 | 84.769 | 20.657 | 1.00 | 38.76 | 6 |
| | ATOM | 203 | O | ALA | B | 287 | -34.882 | 85.193 | 21.814 | 1.00 | 41.98 | 8 |
| | ATOM | 204 | N | LYS | B | 288 | -35.820 | 84.912 | 19.779 | 1.00 | 38.28 | 7 |
| 55 | ATOM | 205 | CA | LYS | B | 288 | -37.066 | 85.584 | 20.112 | 1.00 | 45.26 | 6 |
| | ATOM | 206 | CB | LYS | B | 288 | -37.983 | 85.690 | 18.898 | 1.00 | 48.35 | 6 |
| | ATOM | 207 | CG | LYS | B | 288 | -37.577 | 86.756 | 17.916 | 1.00 | 51.43 | 6 |
| | ATOM | 208 | CD | LYS | B | 288 | -38.806 | 87.359 | 17.226 | 1.00 | 60.23 | 6 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 209 | CE | LYS | B | 288 | -39.680 | 86.308 | 16.564 | 1.00 | 62.81 | 6 |
| | ATOM | 210 | NZ | LYS | B | 288 | -38.897 | 85.460 | 15.614 | 1.00 | 64.69 | 7 |
| | ATOM | 211 | C | LYS | B | 288 | -37.846 | 84.901 | 21.191 | 1.00 | 43.31 | 6 |
| | ATOM | 212 | O | LYS | B | 288 | -38.650 | 85.532 | 21.857 | 1.00 | 45.66 | 8 |
| | ATOM | 213 | N | LYS | B | 289 | -37.618 | 83.604 | 21.345 | 1.00 | 41.70 | 7 |
| 10 | ATOM | 214 | CA | LYS | B | 289 | -38.313 | 82.849 | 22.351 | 1.00 | 40.67 | 6 |
| | ATOM | 215 | CB | LYS | B | 289 | -38.554 | 81.418 | 21.845 | 1.00 | 42.25 | 6 |
| | ATOM | 216 | CG | LYS | B | 289 | -39.438 | 81.368 | 20.589 | 1.00 | 39.53 | 6 |
| | ATOM | 217 | CD | LYS | B | 289 | -40.093 | 80.010 | 20.422 | 1.00 | 43.19 | 6 |
| | ATOM | 218 | CE | LYS | B | 289 | -41.025 | 79.987 | 19.223 | 1.00 | 45.74 | 6 |
| 15 | ATOM | 219 | NZ | LYS | B | 289 | -42.391 | 80.476 | 19.512 | 1.00 | 52.49 | 7 |
| | ATOM | 220 | C | LYS | B | 289 | -37.555 | 82.871 | 23.668 | 1.00 | 41.50 | 6 |
| | ATOM | 221 | O | LYS | B | 289 | -38.057 | 82.366 | 24.657 | 1.00 | 39.77 | 8 |
| | ATOM | 222 | N | LEU | B | 290 | -36.365 | 83.482 | 23.661 | 1.00 | 40.68 | 7 |
| | ATOM | 223 | CA | LEU | B | 290 | -35.539 | 83.599 | 24.854 | 1.00 | 39.33 | 6 |
| 20 | ATOM | 224 | CB | LEU | B | 290 | -34.053 | 83.499 | 24.491 | 1.00 | 36.14 | 6 |
| | ATOM | 225 | CG | LEU | B | 290 | -33.640 | 82.240 | 23.767 | 1.00 | 34.81 | 6 |
| | ATOM | 226 | CD1 | LEU | B | 290 | -32.147 | 82.255 | 23.523 | 1.00 | 29.07 | 6 |
| | ATOM | 227 | CD2 | LEU | B | 290 | -34.013 | 81.040 | 24.607 | 1.00 | 33.45 | 6 |
| | ATOM | 228 | C | LEU | B | 290 | -35.832 | 84.915 | 25.577 | 1.00 | 40.08 | 6 |
| 25 | ATOM | 229 | O | LEU | B | 290 | -35.479 | 86.006 | 25.088 | 1.00 | 42.00 | 8 |
| | ATOM | 230 | N | PRO | B | 291 | -36.462 | 84.840 | 26.765 | 1.00 | 40.27 | 7 |
| | ATOM | 231 | CD | PRO | B | 291 | -36.819 | 83.613 | 27.494 | 1.00 | 39.65 | 6 |
| | ATOM | 232 | CA | PRO | B | 291 | -36.782 | 86.069 | 27.501 | 1.00 | 38.28 | 6 |
| | ATOM | 233 | CB | PRO | B | 291 | -37.376 | 85.574 | 28.811 | 1.00 | 35.88 | 6 |
| 30 | ATOM | 234 | CG | PRO | B | 291 | -37.549 | 84.110 | 28.695 | 1.00 | 34.19 | 6 |
| | ATOM | 235 | C | PRO | B | 291 | -35.570 | 87.002 | 27.714 | 1.00 | 40.05 | 6 |
| | ATOM | 236 | O | PRO | B | 291 | -35.625 | 88.197 | 27.403 | 1.00 | 41.33 | 8 |
| | ATOM | 237 | N | MET | B | 292 | -34.474 | 86.476 | 28.258 | 1.00 | 40.59 | 7 |
| | ATOM | 238 | CA | MET | B | 292 | -33.296 | 87.286 | 28.545 | 1.00 | 42.86 | 6 |
| 35 | ATOM | 239 | CB | MET | B | 292 | -32.149 | 86.376 | 28.975 | 1.00 | 43.28 | 6 |
| | ATOM | 240 | CG | MET | B | 292 | -32.553 | 85.302 | 29.970 | 1.00 | 50.35 | 6 |
| | ATOM | 241 | SD | MET | B | 292 | -31.070 | 84.609 | 30.755 | 1.00 | 51.17 | 16 |
| | ATOM | 242 | CE | MET | B | 292 | -31.797 | 83.212 | 31.701 | 1.00 | 54.63 | 6 |
| | ATOM | 243 | C | MET | B | 292 | -32.895 | 88.077 | 27.315 | 1.00 | 41.05 | 6 |
| 40 | ATOM | 244 | O | MET | B | 292 | -32.228 | 89.098 | 27.420 | 1.00 | 39.66 | 8 |
| | ATOM | 245 | N | PHE | B | 293 | -33.322 | 87.604 | 26.143 | 1.00 | 39.30 | 7 |
| | ATOM | 246 | CA | PHE | B | 293 | -33.017 | 88.271 | 24.878 | 1.00 | 40.92 | 6 |
| | ATOM | 247 | CB | PHE | B | 293 | -33.296 | 87.329 | 23.707 | 1.00 | 40.98 | 6 |
| | ATOM | 248 | CG | PHE | B | 293 | -32.937 | 87.909 | 22.365 | 1.00 | 42.78 | 6 |
| 45 | ATOM | 249 | CD1 | PHE | B | 293 | -31.653 | 88.354 | 22.120 | 1.00 | 44.40 | 6 |
| | ATOM | 250 | CD2 | PHE | B | 293 | -33.872 | 87.972 | 21.350 | 1.00 | 43.66 | 6 |
| | ATOM | 251 | CE1 | PHE | B | 293 | -31.306 | 88.869 | 20.872 | 1.00 | 39.83 | 6 |
| | ATOM | 252 | CE2 | PHE | B | 293 | -33.525 | 88.486 | 20.100 | 1.00 | 46.21 | 6 |
| | ATOM | 253 | CZ | PHE | B | 293 | -32.239 | 88.926 | 19.859 | 1.00 | 45.18 | 6 |
| 50 | ATOM | 254 | C | PHE | B | 293 | -33.873 | 89.518 | 24.744 | 1.00 | 45.54 | 6 |
| | ATOM | 255 | O | PHE | B | 293 | -33.369 | 90.626 | 24.579 | 1.00 | 42.01 | 8 |
| | ATOM | 256 | N | CYS | B | 294 | -35.181 | 89.305 | 24.808 | 1.00 | 47.05 | 7 |
| | ATOM | 257 | CA | CYS | B | 294 | -36.146 | 90.382 | 24.689 | 1.00 | 50.15 | 6 |
| | ATOM | 258 | CB | CYS | B | 294 | -37.553 | 89.793 | 24.756 | 1.00 | 45.90 | 6 |
| 55 | ATOM | 259 | SG | CYS | B | 294 | -37.899 | 88.607 | 23.449 | 1.00 | 51.50 | 16 |
| | ATOM | 260 | C | CYS | B | 294 | -35.974 | 91.474 | 25.751 | 1.00 | 51.38 | 6 |
| | ATOM | 261 | O | CYS | B | 294 | -36.585 | 92.536 | 25.656 | 1.00 | 53.83 | 8 |
| | ATOM | 262 | N | GLU | B | 295 | -35.137 | 91.200 | 26.753 | 1.00 | 49.72 | 7 |

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|----|------|-----|-----|-----------|---------|---------|--------|------|-------|----|
| 5 | ATOM | 263 | CA | GLU B 295 | -34.839 | 92.159 | 27.816 | 1.00 | 52.53 | 6 |
| | ATOM | 264 | CB | GLU B 295 | -34.553 | 91.412 | 29.131 | 1.00 | 57.40 | 6 |
| | ATOM | 265 | CG | GLU B 295 | -35.811 | 90.978 | 29.874 | 1.00 | 69.63 | 6 |
| | ATOM | 266 | CD | GLU B 295 | -36.610 | 92.144 | 30.375 | 1.00 | 78.49 | 6 |
| | ATOM | 267 | OE1 | GLU B 295 | -36.153 | 92.869 | 31.297 | 1.00 | 82.82 | 8 |
| 10 | ATOM | 268 | OE2 | GLU B 295 | -37.730 | 92.385 | 29.860 | 1.00 | 85.30 | 8 |
| | ATOM | 269 | C | GLU B 295 | -33.629 | 93.009 | 27.415 | 1.00 | 48.54 | 6 |
| | ATOM | 270 | O | GLU B 295 | -32.981 | 93.627 | 28.260 | 1.00 | 49.82 | 8 |
| | ATOM | 271 | N | LEU B 296 | -33.374 | 93.030 | 26.109 | 1.00 | 43.79 | 7 |
| | ATOM | 272 | CA | LEU B 296 | -32.268 | 93.761 | 25.540 | 1.00 | 45.42 | 6 |
| 15 | ATOM | 273 | CB | LEU B 296 | -31.319 | 92.769 | 24.838 | 1.00 | 41.04 | 6 |
| | ATOM | 274 | CG | LEU B 296 | -30.735 | 91.631 | 25.662 | 1.00 | 42.74 | 6 |
| | ATOM | 275 | CD1 | LEU B 296 | -30.354 | 90.478 | 24.764 | 1.00 | 40.99 | 6 |
| | ATOM | 276 | CD2 | LEU B 296 | -29.559 | 92.119 | 26.468 | 1.00 | 39.44 | 6 |
| | ATOM | 277 | C | LEU B 296 | -32.760 | 94.779 | 24.522 | 1.00 | 45.56 | 6 |
| 20 | ATOM | 278 | O | LEU B 296 | -33.845 | 94.600 | 23.924 | 1.00 | 43.07 | 8 |
| | ATOM | 279 | N | PRO B 297 | -32.004 | 95.875 | 24.338 | 1.00 | 46.99 | 7 |
| | ATOM | 280 | CD | PRO B 297 | -30.740 | 96.123 | 25.046 | 1.00 | 47.12 | 6 |
| | ATOM | 281 | CA | PRO B 297 | -32.388 | 96.912 | 23.363 | 1.00 | 49.61 | 6 |
| | ATOM | 282 | CB | PRO B 297 | -31.294 | 97.973 | 23.494 | 1.00 | 49.91 | 6 |
| 25 | ATOM | 283 | CG | PRO B 297 | -30.302 | 97.477 | 24.545 | 1.00 | 51.28 | 6 |
| | ATOM | 284 | C | PRO B 297 | -32.263 | 96.273 | 21.913 | 1.00 | 49.59 | 6 |
| | ATOM | 285 | O | PRO B 297 | -31.441 | 95.340 | 21.685 | 1.00 | 51.66 | 8 |
| | ATOM | 286 | N | CYS B 298 | -33.035 | 96.667 | 20.854 | 1.00 | 51.02 | 7 |
| | ATOM | 287 | CA | CYS B 298 | -32.761 | 96.150 | 19.456 | 1.00 | 52.86 | 6 |
| 30 | ATOM | 288 | CB | CYS B 298 | -33.140 | 97.165 | 18.356 | 1.00 | 54.57 | 6 |
| | ATOM | 289 | SG | CYS B 298 | -34.884 | 97.085 | 17.836 | 1.00 | 67.87 | 16 |
| | ATOM | 290 | C | CYS B 298 | -31.385 | 96.330 | 19.127 | 1.00 | 48.51 | 6 |
| | ATOM | 291 | O | CYS B 298 | -30.579 | 95.506 | 18.744 | 1.00 | 49.58 | 8 |
| | ATOM | 292 | N | GLU B 299 | -31.107 | 97.447 | 19.230 | 1.00 | 44.17 | 7 |
| 35 | ATOM | 293 | CA | GLU B 299 | -29.989 | 97.645 | 18.718 | 1.00 | 47.57 | 6 |
| | ATOM | 294 | CB | GLU B 299 | -29.402 | 98.973 | 19.208 | 1.00 | 49.92 | 6 |
| | ATOM | 295 | CG | GLU B 299 | -29.944 | 100.187 | 18.433 | 1.00 | 59.30 | 6 |
| | ATOM | 296 | CD | GLU B 299 | -31.090 | 100.887 | 19.164 | 1.00 | 63.80 | 6 |
| | ATOM | 297 | OE1 | GLU B 299 | -31.673 | 101.904 | 18.629 | 1.00 | 69.03 | 8 |
| 40 | ATOM | 298 | OE2 | GLU B 299 | -31.473 | 100.458 | 20.319 | 1.00 | 67.10 | 8 |
| | ATOM | 299 | C | GLU B 299 | -28.993 | 96.533 | 18.987 | 1.00 | 46.57 | 6 |
| | ATOM | 300 | O | GLU B 299 | -28.200 | 96.179 | 18.111 | 1.00 | 44.65 | 8 |
| | ATOM | 301 | N | ASP B 300 | -29.045 | 95.989 | 20.203 | 1.00 | 45.17 | 7 |
| | ATOM | 302 | CA | ASP B 300 | -28.152 | 94.908 | 20.584 | 1.00 | 43.32 | 6 |
| 45 | ATOM | 303 | CB | ASP B 300 | -27.985 | 94.849 | 22.105 | 1.00 | 37.38 | 6 |
| | ATOM | 304 | CG | ASP B 300 | -27.239 | 96.016 | 22.650 | 1.00 | 36.23 | 6 |
| | ATOM | 305 | OD1 | ASP B 300 | -26.208 | 96.421 | 22.052 | 1.00 | 35.87 | 8 |
| | ATOM | 306 | OD2 | ASP B 300 | -27.661 | 96.543 | 23.716 | 1.00 | 40.14 | 8 |
| | ATOM | 307 | C | ASP B 300 | -28.721 | 93.591 | 20.071 | 1.00 | 42.81 | 6 |
| 50 | ATOM | 308 | O | ASP B 300 | -28.001 | 92.775 | 19.489 | 1.00 | 46.02 | 8 |
| | ATOM | 309 | N | GLN B 301 | -30.019 | 93.399 | 20.306 | 1.00 | 38.60 | 7 |
| | ATOM | 310 | CA | GLN B 301 | -30.712 | 92.197 | 19.858 | 1.00 | 40.00 | 6 |
| | ATOM | 311 | CB | GLN B 301 | -32.234 | 92.418 | 19.836 | 1.00 | 38.59 | 6 |
| | ATOM | 312 | CG | GLN B 301 | -32.908 | 92.380 | 21.187 | 1.00 | 40.26 | 6 |
| 55 | ATOM | 313 | CD | GLN B 301 | -34.401 | 92.583 | 21.083 | 1.00 | 44.15 | 6 |
| | ATOM | 314 | OE1 | GLN B 301 | -34.859 | 93.637 | 20.589 | 1.00 | 45.73 | 8 |
| | ATOM | 315 | NE2 | GLN B 301 | -35.165 | 91.602 | 21.544 | 1.00 | 46.13 | 7 |
| | ATOM | 316 | C | GLN B 301 | -30.237 | 91.830 | 18.455 | 1.00 | 41.64 | 6 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 317 | O | GLN | B | 301 | -30.162 | 90.662 | 18.100 | 1.00 | 45.02 | 8. |
| | ATOM | 318 | N | ILE | B | 302 | -29.916 | 92.864 | 17.674 | 1.00 | 41.01 | 7 |
| | ATOM | 319 | CA | ILE | B | 302 | -29.424 | 92.692 | 16.311 | 1.00 | 40.23 | 6 |
| | ATOM | 320 | CB | ILE | B | 302 | -29.584 | 93.978 | 15.498 | 1.00 | 39.52 | 6 |
| | ATOM | 321 | CG2 | ILE | B | 302 | -29.034 | 93.792 | 14.100 | 1.00 | 31.98 | 6 |
| 10 | ATOM | 322 | CG1 | ILE | B | 302 | -31.059 | 94.385 | 15.416 | 1.00 | 40.77 | 6 |
| | ATOM | 323 | CD1 | ILE | B | 302 | -31.939 | 93.317 | 14.775 | 1.00 | 45.43 | 6 |
| | ATOM | 324 | C | ILE | B | 302 | -27.966 | 92.260 | 16.342 | 1.00 | 38.58 | 6 |
| | ATOM | 325 | O | ILE | B | 302 | -27.613 | 91.197 | 15.830 | 1.00 | 40.81 | 8 |
| | ATOM | 326 | N | ILE | B | 303 | -27.128 | 93.111 | 16.933 | 1.00 | 37.50 | 7 |
| 15 | ATOM | 327 | CA | ILE | B | 303 | -25.692 | 92.846 | 17.062 | 1.00 | 39.33 | 6 |
| | ATOM | 328 | CB | ILE | B | 303 | -25.066 | 93.648 | 18.203 | 1.00 | 39.06 | 6 |
| | ATOM | 329 | CG2 | ILE | B | 303 | -23.566 | 93.405 | 18.257 | 1.00 | 36.19 | 6 |
| | ATOM | 330 | CG1 | ILE | B | 303 | -25.309 | 95.143 | 18.020 | 1.00 | 40.15 | 6 |
| | ATOM | 331 | CD1 | ILE | B | 303 | -24.816 | 95.966 | 19.173 | 1.00 | 36.93 | 6 |
| 20 | ATOM | 332 | C | ILE | B | 303 | -25.470 | 91.365 | 17.323 | 1.00 | 36.49 | 6 |
| | ATOM | 333 | O | ILE | B | 303 | -24.619 | 90.725 | 16.712 | 1.00 | 36.58 | 8 |
| | ATOM | 334 | N | LEU | B | 304 | -26.244 | 90.843 | 18.266 | 1.00 | 32.91 | 7 |
| | ATOM | 335 | CA | LEU | B | 304 | -26.194 | 89.433 | 18.633 | 1.00 | 27.55 | 6 |
| | ATOM | 336 | CB | LEU | B | 304 | -27.172 | 89.182 | 19.793 | 1.00 | 22.35 | 6 |
| 25 | ATOM | 337 | CG | LEU | B | 304 | -26.623 | 89.449 | 21.187 | 1.00 | 26.88 | 6 |
| | ATOM | 338 | CD1 | LEU | B | 304 | -25.540 | 90.495 | 21.136 | 1.00 | 24.82 | 6 |
| | ATOM | 339 | CD2 | LEU | B | 304 | -27.747 | 89.840 | 22.121 | 1.00 | 23.69 | 6 |
| | ATOM | 340 | C | LEU | B | 304 | -26.505 | 88.547 | 17.425 | 1.00 | 28.05 | 6 |
| | ATOM | 341 | O | LEU | B | 304 | -25.668 | 87.751 | 16.983 | 1.00 | 24.68 | 8 |
| 30 | ATOM | 342 | N | LEU | B | 305 | -27.716 | 88.700 | 16.897 | 1.00 | 26.34 | 7 |
| | ATOM | 343 | CA | LEU | B | 305 | -28.145 | 87.939 | 15.741 | 1.00 | 30.91 | 6 |
| | ATOM | 344 | CB | LEU | B | 305 | -29.460 | 88.514 | 15.199 | 1.00 | 32.50 | 6 |
| | ATOM | 345 | CG | LEU | B | 305 | -30.699 | 88.305 | 16.050 | 1.00 | 33.36 | 6 |
| | ATOM | 346 | CD1 | LEU | B | 305 | -31.938 | 88.839 | 15.342 | 1.00 | 33.87 | 6 |
| 35 | ATOM | 347 | CD2 | LEU | B | 305 | -30.863 | 86.812 | 16.298 | 1.00 | 31.72 | 6 |
| | ATOM | 348 | C | LEU | B | 305 | -27.072 | 87.922 | 14.666 | 1.00 | 29.76 | 6 |
| | ATOM | 349 | O | LEU | B | 305 | -26.687 | 86.860 | 14.202 | 1.00 | 29.33 | 8 |
| | ATOM | 350 | N | LYS | B | 306 | -26.597 | 89.107 | 14.291 | 1.00 | 29.72 | 7 |
| | ATOM | 351 | CA | LYS | B | 306 | -25.576 | 89.254 | 13.264 | 1.00 | 34.28 | 6 |
| 40 | ATOM | 352 | CB | LYS | B | 306 | -25.224 | 90.732 | 13.077 | 1.00 | 35.98 | 6 |
| | ATOM | 353 | CG | LYS | B | 306 | -26.350 | 91.581 | 12.494 | 1.00 | 43.35 | 6 |
| | ATOM | 354 | CD | LYS | B | 306 | -25.852 | 92.987 | 12.182 | 1.00 | 51.50 | 6 |
| | ATOM | 355 | CE | LYS | B | 306 | -24.706 | 92.932 | 11.190 | 1.00 | 53.26 | 6 |
| | ATOM | 356 | NZ | LYS | B | 306 | -23.883 | 94.161 | 11.251 | 1.00 | 59.61 | 7 |
| 45 | ATOM | 357 | C | LYS | B | 306 | -24.308 | 88.484 | 13.556 | 1.00 | 35.25 | 6 |
| | ATOM | 358 | O | LYS | B | 306 | -23.681 | 87.917 | 12.653 | 1.00 | 33.95 | 8 |
| | ATOM | 359 | N | GLY | B | 307 | -23.918 | 88.478 | 14.829 | 1.00 | 35.79 | 7 |
| | ATOM | 360 | CA | GLY | B | 307 | -22.702 | 87.793 | 15.227 | 1.00 | 34.59 | 6 |
| | ATOM | 361 | C | GLY | B | 307 | -22.811 | 86.291 | 15.383 | 1.00 | 33.80 | 6 |
| 50 | ATOM | 362 | O | GLY | B | 307 | -21.944 | 85.564 | 14.895 | 1.00 | 31.59 | 8 |
| | ATOM | 363 | N | CYS | B | 308 | -23.861 | 85.843 | 16.071 | 1.00 | 31.15 | 7 |
| | ATOM | 364 | CA | CYS | B | 308 | -24.069 | 84.434 | 16.320 | 1.00 | 29.04 | 6 |
| | ATOM | 365 | CB | CYS | B | 308 | -24.761 | 84.240 | 17.663 | 1.00 | 27.59 | 6 |
| | ATOM | 366 | SG | CYS | B | 308 | -26.496 | 84.629 | 17.608 | 1.00 | 30.50 | 16 |
| 55 | ATOM | 367 | C | CYS | B | 308 | -24.911 | 83.712 | 15.266 | 1.00 | 30.59 | 6 |
| | ATOM | 368 | O | CYS | B | 308 | -25.088 | 82.499 | 15.365 | 1.00 | 33.77 | 8 |
| | ATOM | 369 | N | CYS | B | 309 | -25.432 | 84.429 | 14.266 | 1.00 | 28.46 | 7 |
| | ATOM | 370 | CA | CYS | B | 309 | -26.270 | 83.787 | 13.265 | 1.00 | 30.10 | 6 |

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|----|------|-----|-----|-----------|---------|--------|--------|------|-------|----|
| 5 | ATOM | 371 | CB | CYS B 309 | -26.706 | 84.761 | 12.194 | 1.00 | 33.43 | 6 |
| | ATOM | 372 | SG | CYS B 309 | -27.875 | 84.011 | 11.089 | 1.00 | 35.20 | 16 |
| | ATOM | 373 | C | CYS B 309 | -25.617 | 82.608 | 12.603 | 1.00 | 27.72 | 6 |
| | ATOM | 374 | O | CYS B 309 | -26.170 | 81.518 | 12.610 | 1.00 | 27.69 | 8 |
| | ATOM | 375 | N | MET B 310 | -24.447 | 82.829 | 12.011 | 1.00 | 26.15 | 7 |
| 10 | ATOM | 376 | CA | MET B 310 | -23.737 | 81.748 | 11.352 | 1.00 | 26.06 | 6 |
| | ATOM | 377 | CB | MET B 310 | -22.439 | 82.263 | 10.712 | 1.00 | 25.32 | 6 |
| | ATOM | 378 | CG | MET B 310 | -21.584 | 81.157 | 10.080 | 1.00 | 24.08 | 6 |
| | ATOM | 379 | SD | MET B 310 | -22.555 | 80.324 | 8.758 | 1.00 | 27.71 | 16 |
| | ATOM | 380 | CE | MET B 310 | -21.549 | 78.826 | 8.427 | 1.00 | 28.50 | 6 |
| 15 | ATOM | 381 | C | MET B 310 | -23.416 | 80.673 | 12.374 | 1.00 | 25.94 | 6 |
| | ATOM | 382 | O | MET B 310 | -23.659 | 79.489 | 12.151 | 1.00 | 28.09 | 8 |
| | ATOM | 383 | N | GLU B 311 | -22.865 | 81.117 | 13.500 | 1.00 | 25.39 | 7 |
| | ATOM | 384 | CA | GLU B 311 | -22.466 | 80.231 | 14.576 | 1.00 | 27.03 | 6 |
| | ATOM | 385 | CB | GLU B 311 | -22.036 | 81.048 | 15.797 | 1.00 | 24.39 | 6 |
| 20 | ATOM | 386 | CG | GLU B 311 | -21.019 | 82.141 | 15.509 | 1.00 | 26.00 | 6 |
| | ATOM | 387 | CD | GLU B 311 | -20.524 | 82.835 | 16.740 | 1.00 | 23.95 | 6 |
| | ATOM | 388 | OE1 | GLU B 311 | -21.321 | 83.108 | 17.668 | 1.00 | 19.72 | 8 |
| | ATOM | 389 | OE2 | GLU B 311 | -19.313 | 83.163 | 16.815 | 1.00 | 26.51 | 8 |
| | ATOM | 390 | C | GLU B 311 | -23.582 | 79.264 | 14.964 | 1.00 | 27.51 | 6 |
| 25 | ATOM | 391 | O | GLU B 311 | -23.347 | 78.068 | 15.093 | 1.00 | 29.67 | 8 |
| | ATOM | 392 | N | ILE B 312 | -24.794 | 79.792 | 15.145 | 1.00 | 26.82 | 7 |
| | ATOM | 393 | CA | ILE B 312 | -25.933 | 78.967 | 15.527 | 1.00 | 25.71 | 6 |
| | ATOM | 394 | CB | ILE B 312 | -27.125 | 79.814 | 16.021 | 1.00 | 23.35 | 6 |
| | ATOM | 395 | CG2 | ILE B 312 | -28.327 | 78.933 | 16.276 | 1.00 | 20.27 | 6 |
| 30 | ATOM | 396 | CG1 | ILE B 312 | -26.771 | 80.541 | 17.325 | 1.00 | 20.88 | 6 |
| | ATOM | 397 | CD1 | ILE B 312 | -27.952 | 81.163 | 18.028 | 1.00 | 18.15 | 6 |
| | ATOM | 398 | C | ILE B 312 | -26.370 | 78.072 | 14.392 | 1.00 | 27.91 | 6 |
| | ATOM | 399 | O | ILE B 312 | -26.769 | 76.926 | 14.605 | 1.00 | 28.96 | 8 |
| | ATOM | 400 | N | MET B 313 | -26.303 | 78.603 | 13.174 | 1.00 | 27.66 | 7 |
| 35 | ATOM | 401 | CA | MET B 313 | -26.696 | 77.832 | 11.999 | 1.00 | 30.18 | 6 |
| | ATOM | 402 | CB | MET B 313 | -26.696 | 78.691 | 10.734 | 1.00 | 36.89 | 6 |
| | ATOM | 403 | CG | MET B 313 | -27.882 | 79.634 | 10.607 | 1.00 | 37.95 | 6 |
| | ATOM | 404 | SD | MET B 313 | -28.238 | 80.275 | 8.907 | 1.00 | 42.38 | 16 |
| | ATOM | 405 | CE | MET B 313 | -26.787 | 81.316 | 8.639 | 1.00 | 40.68 | 6 |
| 40 | ATOM | 406 | C | MET B 313 | -25.791 | 76.632 | 11.808 | 1.00 | 27.43 | 6 |
| | ATOM | 407 | O | MET B 313 | -26.258 | 75.501 | 11.893 | 1.00 | 28.61 | 8 |
| | ATOM | 408 | N | SER B 314 | -24.508 | 76.882 | 11.549 | 1.00 | 24.88 | 7 |
| | ATOM | 409 | CA | SER B 314 | -23.533 | 75.824 | 11.346 | 1.00 | 27.98 | 6 |
| | ATOM | 410 | CB | SER B 314 | -22.150 | 76.441 | 11.165 | 1.00 | 29.64 | 6 |
| 45 | ATOM | 411 | OG | SER B 314 | -21.844 | 77.316 | 12.227 | 1.00 | 43.44 | 8 |
| | ATOM | 412 | C | SER B 314 | -23.514 | 74.774 | 12.465 | 1.00 | 22.30 | 6 |
| | ATOM | 413 | O | SER B 314 | -23.279 | 73.592 | 12.199 | 1.00 | 24.18 | 8 |
| | ATOM | 414 | N | LEU B 315 | -23.760 | 75.187 | 13.714 | 1.00 | 23.99 | 7 |
| | ATOM | 415 | CA | LEU B 315 | -23.792 | 74.219 | 14.811 | 1.00 | 25.07 | 6 |
| 50 | ATOM | 416 | CB | LEU B 315 | -24.095 | 74.869 | 16.169 | 1.00 | 19.11 | 6 |
| | ATOM | 417 | CG | LEU B 315 | -24.507 | 73.860 | 17.234 | 1.00 | 20.39 | 6 |
| | ATOM | 418 | CD1 | LEU B 315 | -23.390 | 72.878 | 17.493 | 1.00 | 18.92 | 6 |
| | ATOM | 419 | CD2 | LEU B 315 | -24.895 | 74.560 | 18.514 | 1.00 | 12.93 | 6 |
| | ATOM | 420 | C | LEU B 315 | -24.892 | 73.219 | 14.517 | 1.00 | 24.53 | 6 |
| 55 | ATOM | 421 | O | LEU B 315 | -24.672 | 72.014 | 14.550 | 1.00 | 26.32 | 8 |
| | ATOM | 422 | N | ARG B 316 | -26.079 | 73.762 | 14.254 | 1.00 | 28.18 | 7 |
| | ATOM | 423 | CA | ARG B 316 | -27.278 | 72.996 | 13.971 | 1.00 | 27.54 | 6 |
| | ATOM | 424 | CB | ARG B 316 | -28.432 | 73.941 | 13.651 | 1.00 | 27.39 | 6 |

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|----|------|-----|-----|-----------|---------|--------|--------|------|-------|---|
| 5 | ATOM | 425 | CG | ARG B 316 | -28.823 | 74.857 | 14.809 | 1.00 | 22.00 | 6 |
| | ATOM | 426 | CD | ARG B 316 | -30.074 | 75.657 | 14.451 | 1.00 | 18.78 | 6 |
| | ATOM | 427 | NE | ARG B 316 | -30.905 | 75.944 | 15.598 | 1.00 | 26.57 | 7 |
| | ATOM | 428 | CZ | ARG B 316 | -32.166 | 76.337 | 15.489 | 1.00 | 30.81 | 6 |
| | ATOM | 429 | NH1 | ARG B 316 | -32.686 | 76.535 | 14.280 | 1.00 | 33.71 | 7 |
| 10 | ATOM | 430 | NH2 | ARG B 316 | -32.900 | 76.542 | 16.581 | 1.00 | 33.13 | 7 |
| | ATOM | 431 | C | ARG B 316 | -27.128 | 72.028 | 12.830 | 1.00 | 28.09 | 6 |
| | ATOM | 432 | O | ARG B 316 | -27.852 | 71.053 | 12.760 | 1.00 | 32.41 | 8 |
| | ATOM | 433 | N | ALA B 317 | -26.187 | 72.309 | 11.941 | 1.00 | 28.36 | 7 |
| | ATOM | 434 | CA | ALA B 317 | -25.938 | 71.466 | 10.794 | 1.00 | 26.64 | 6 |
| 15 | ATOM | 435 | CB | ALA B 317 | -25.337 | 72.300 | 9.675 | 1.00 | 22.93 | 6 |
| | ATOM | 436 | C | ALA B 317 | -24.998 | 70.327 | 11.150 | 1.00 | 28.35 | 6 |
| | ATOM | 437 | O | ALA B 317 | -25.223 | 69.187 | 10.773 | 1.00 | 32.10 | 8 |
| | ATOM | 438 | N | ALA B 318 | -23.941 | 70.659 | 11.882 | 1.00 | 29.12 | 7 |
| | ATOM | 439 | CA | ALA B 318 | -22.957 | 69.682 | 12.299 | 1.00 | 27.50 | 6 |
| 20 | ATOM | 440 | CB | ALA B 318 | -21.915 | 70.355 | 13.160 | 1.00 | 28.39 | 6 |
| | ATOM | 441 | C | ALA B 318 | -23.645 | 68.591 | 13.084 | 1.00 | 28.10 | 6 |
| | ATOM | 442 | O | ALA B 318 | -23.415 | 67.415 | 12.854 | 1.00 | 28.18 | 8 |
| | ATOM | 443 | N | VAL B 319 | -24.502 | 69.012 | 14.016 | 1.00 | 29.16 | 7 |
| | ATOM | 444 | CA | VAL B 319 | -25.259 | 68.107 | 14.889 | 1.00 | 35.24 | 6 |
| 25 | ATOM | 445 | CB | VAL B 319 | -26.228 | 68.897 | 15.765 | 1.00 | 27.34 | 6 |
| | ATOM | 446 | CG1 | VAL B 319 | -25.576 | 70.149 | 16.246 | 1.00 | 29.96 | 6 |
| | ATOM | 447 | CG2 | VAL B 319 | -27.505 | 69.212 | 15.022 | 1.00 | 31.70 | 6 |
| | ATOM | 448 | C | VAL B 319 | -26.066 | 67.146 | 14.043 | 1.00 | 40.01 | 6 |
| | ATOM | 449 | O | VAL B 319 | -26.701 | 66.250 | 14.578 | 1.00 | 42.70 | 8 |
| 30 | ATOM | 450 | N | ARG B 320 | -26.025 | 67.353 | 12.723 | 1.00 | 38.64 | 7 |
| | ATOM | 451 | CA | ARG B 320 | -26.770 | 66.541 | 11.762 | 1.00 | 38.61 | 6 |
| | ATOM | 452 | CB | ARG B 320 | -27.838 | 67.409 | 11.123 | 1.00 | 37.26 | 6 |
| | ATOM | 453 | CG | ARG B 320 | -29.152 | 67.280 | 11.822 | 1.00 | 43.12 | 6 |
| | ATOM | 454 | CD | ARG B 320 | -30.145 | 68.340 | 11.387 | 1.00 | 50.79 | 6 |
| 35 | ATOM | 455 | NE | ARG B 320 | -31.500 | 67.911 | 11.705 | 1.00 | 54.71 | 7 |
| | ATOM | 456 | CZ | ARG B 320 | -32.555 | 68.723 | 11.597 | 1.00 | 57.89 | 6 |
| | ATOM | 457 | NH1 | ARG B 320 | -32.398 | 69.957 | 11.130 | 1.00 | 49.08 | 7 |
| | ATOM | 458 | NH2 | ARG B 320 | -33.773 | 68.302 | 11.844 | 1.00 | 59.59 | 7 |
| | ATOM | 459 | C | ARG B 320 | -25.937 | 65.910 | 10.670 | 1.00 | 42.14 | 6 |
| 40 | ATOM | 460 | O | ARG B 320 | -26.381 | 65.802 | 9.532 | 1.00 | 46.30 | 8 |
| | ATOM | 461 | N | TYR B 321 | -24.734 | 65.488 | 11.022 | 1.00 | 42.04 | 7 |
| | ATOM | 462 | CA | TYR B 321 | -23.858 | 64.848 | 10.063 | 1.00 | 42.70 | 6 |
| | ATOM | 463 | CB | TYR B 321 | -22.433 | 65.332 | 10.297 | 1.00 | 38.01 | 6 |
| | ATOM | 464 | CG | TYR B 321 | -21.393 | 64.396 | 9.756 | 1.00 | 37.94 | 6 |
| 45 | ATOM | 465 | CD1 | TYR B 321 | -21.265 | 64.176 | 8.397 | 1.00 | 33.85 | 6 |
| | ATOM | 466 | CE1 | TYR B 321 | -20.333 | 63.258 | 7.912 | 1.00 | 34.49 | 6 |
| | ATOM | 467 | CD2 | TYR B 321 | -20.583 | 63.683 | 10.613 | 1.00 | 28.03 | 6 |
| | ATOM | 468 | CE2 | TYR B 321 | -19.658 | 62.769 | 10.134 | 1.00 | 32.69 | 6 |
| | ATOM | 469 | CZ | TYR B 321 | -19.532 | 62.551 | 8.781 | 1.00 | 35.18 | 6 |
| 50 | ATOM | 470 | OH | TYR B 321 | -18.616 | 61.661 | 8.292 | 1.00 | 39.48 | 8 |
| | ATOM | 471 | C | TYR B 321 | -23.897 | 63.347 | 10.234 | 1.00 | 45.51 | 6 |
| | ATOM | 472 | O | TYR B 321 | -23.560 | 62.857 | 11.292 | 1.00 | 48.02 | 8 |
| | ATOM | 473 | N | ASP B 322 | -24.317 | 62.642 | 9.188 | 1.00 | 44.56 | 7 |
| | ATOM | 474 | CA | ASP B 322 | -24.391 | 61.170 | 9.182 | 1.00 | 45.86 | 6 |
| 55 | ATOM | 475 | CB | ASP B 322 | -25.570 | 60.749 | 8.294 | 1.00 | 46.64 | 6 |
| | ATOM | 476 | CG | ASP B 322 | -25.449 | 59.359 | 7.775 | 1.00 | 40.00 | 6 |
| | ATOM | 477 | OD1 | ASP B 322 | -24.388 | 58.737 | 7.986 | 1.00 | 40.00 | 8 |
| | ATOM | 478 | OD2 | ASP B 322 | -26.414 | 58.862 | 7.117 | 1.00 | 40.00 | 8 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 479 | C | ASP | B | 322 | -23.044 | 60.659 | 8.682 | 1.00 | 45.82 | 6 |
| | ATOM | 480 | O | ASP | B | 322 | -22.738 | 60.783 | 7.495 | 1.00 | 45.38 | 8 |
| | ATOM | 481 | N | PRO | B | 323 | -22.242 | 60.005 | 9.549 | 1.00 | 46.53 | 7 |
| | ATOM | 482 | CD | PRO | B | 323 | -22.594 | 59.676 | 10.934 | 1.00 | 47.16 | 6 |
| | ATOM | 483 | CA | PRO | B | 323 | -20.910 | 59.487 | 9.162 | 1.00 | 46.63 | 6 |
| 10 | ATOM | 484 | CB | PRO | B | 323 | -20.367 | 58.847 | 10.433 | 1.00 | 43.95 | 6 |
| | ATOM | 485 | CG | PRO | B | 323 | -21.398 | 58.958 | 11.454 | 1.00 | 43.93 | 6 |
| | ATOM | 486 | C | PRO | B | 323 | -20.933 | 58.489 | 8.017 | 1.00 | 48.34 | 6 |
| | ATOM | 487 | O | PRO | B | 323 | -20.040 | 58.457 | 7.171 | 1.00 | 50.84 | 8 |
| | ATOM | 488 | N | GLU | B | 324 | -21.951 | 57.631 | 8.022 | 1.00 | 52.39 | 7 |
| 15 | ATOM | 489 | CA | GLU | B | 324 | -22.126 | 56.615 | 7.008 | 1.00 | 55.85 | 6 |
| | ATOM | 490 | CB | GLU | B | 324 | -23.491 | 55.960 | 7.216 | 1.00 | 55.54 | 6 |
| | ATOM | 491 | CG | GLU | B | 324 | -23.678 | 55.332 | 8.581 | 1.00 | 40.00 | 6 |
| | ATOM | 492 | CD | GLU | B | 324 | -22.642 | 54.294 | 8.888 | 1.00 | 40.00 | 6 |
| | ATOM | 493 | OE1 | GLU | B | 324 | -21.796 | 53.979 | 8.000 | 1.00 | 40.00 | 8 |
| 20 | ATOM | 494 | OE2 | GLU | B | 324 | -22.645 | 53.751 | 10.029 | 1.00 | 40.00 | 8 |
| | ATOM | 495 | C | GLU | B | 324 | -22.087 | 57.292 | 5.655 | 1.00 | 54.94 | 6 |
| | ATOM | 496 | O | GLU | B | 324 | -21.144 | 57.149 | 4.896 | 1.00 | 59.81 | 8 |
| | ATOM | 497 | N | SER | B | 325 | -23.165 | 58.022 | 5.389 | 1.00 | 52.95 | 7 |
| | ATOM | 498 | CA | SER | B | 325 | -23.358 | 58.762 | 4.163 | 1.00 | 50.10 | 6 |
| 25 | ATOM | 499 | CB | SER | B | 325 | -24.768 | 59.357 | 4.163 | 1.00 | 48.23 | 6 |
| | ATOM | 500 | OG | SER | B | 325 | -25.051 | 59.976 | 5.403 | 1.00 | 48.71 | 8 |
| | ATOM | 501 | C | SER | B | 325 | -22.324 | 59.861 | 3.964 | 1.00 | 50.61 | 6 |
| | ATOM | 502 | O | SER | B | 325 | -21.956 | 60.176 | 2.848 | 1.00 | 52.19 | 8 |
| | ATOM | 503 | N | GLU | B | 326 | -21.851 | 60.422 | 5.070 | 1.00 | 45.64 | 7 |
| 30 | ATOM | 504 | CA | GLU | B | 326 | -20.854 | 61.476 | 5.050 | 1.00 | 43.35 | 6 |
| | ATOM | 505 | CB | GLU | B | 326 | -19.602 | 61.022 | 4.277 | 1.00 | 42.74 | 6 |
| | ATOM | 506 | CG | GLU | B | 326 | -18.880 | 59.814 | 4.876 | 1.00 | 50.32 | 6 |
| | ATOM | 507 | CD | GLU | B | 326 | -17.576 | 59.524 | 4.207 | 1.00 | 56.34 | 6 |
| | ATOM | 508 | OE1 | GLU | B | 326 | -16.898 | 58.545 | 4.608 | 1.00 | 59.31 | 8 |
| 35 | ATOM | 509 | OE2 | GLU | B | 326 | -17.177 | 60.255 | 3.266 | 1.00 | 55.74 | 8 |
| | ATOM | 510 | C | GLU | B | 326 | -21.401 | 62.731 | 4.418 | 1.00 | 40.23 | 6 |
| | ATOM | 511 | O | GLU | B | 326 | -20.793 | 63.285 | 3.514 | 1.00 | 40.44 | 8 |
| | ATOM | 512 | N | THR | B | 327 | -22.528 | 63.208 | 4.934 | 1.00 | 35.90 | 7 |
| | ATOM | 513 | CA | THR | B | 327 | -23.163 | 64.418 | 4.401 | 1.00 | 37.29 | 6 |
| 40 | ATOM | 514 | CB | THR | B | 327 | -24.146 | 64.052 | 3.285 | 1.00 | 37.63 | 6 |
| | ATOM | 515 | OG1 | THR | B | 327 | -25.172 | 63.199 | 3.803 | 1.00 | 38.12 | 8 |
| | ATOM | 516 | CG2 | THR | B | 327 | -23.445 | 63.342 | 2.130 | 1.00 | 39.90 | 6 |
| | ATOM | 517 | C | THR | B | 327 | -23.961 | 65.125 | 5.473 | 1.00 | 39.49 | 6 |
| | ATOM | 518 | O | THR | B | 327 | -24.645 | 64.473 | 6.264 | 1.00 | 40.50 | 8 |
| 45 | ATOM | 519 | N | LEU | B | 328 | -23.909 | 66.454 | 5.473 | 1.00 | 36.64 | 7 |
| | ATOM | 520 | CA | LEU | B | 328 | -24.675 | 67.239 | 6.447 | 1.00 | 37.73 | 6 |
| | ATOM | 521 | CB | LEU | B | 328 | -24.061 | 68.637 | 6.620 | 1.00 | 37.78 | 6 |
| | ATOM | 522 | CG | LEU | B | 328 | -22.586 | 68.750 | 6.931 | 1.00 | 36.26 | 6 |
| | ATOM | 523 | CD1 | LEU | B | 328 | -22.260 | 70.145 | 7.411 | 1.00 | 36.56 | 6 |
| 50 | ATOM | 524 | CD2 | LEU | B | 328 | -22.231 | 67.751 | 8.000 | 1.00 | 39.85 | 6 |
| | ATOM | 525 | C | LEU | B | 328 | -26.090 | 67.344 | 5.897 | 1.00 | 37.27 | 6 |
| | ATOM | 526 | O | LEU | B | 328 | -26.358 | 66.855 | 4.805 | 1.00 | 34.96 | 8 |
| | ATOM | 527 | N | THR | B | 329 | -26.989 | 67.975 | 6.647 | 1.00 | 39.73 | 7 |
| | ATOM | 528 | CA | THR | B | 329 | -28.369 | 68.132 | 6.215 | 1.00 | 40.81 | 6 |
| 55 | ATOM | 529 | CB | THR | B | 329 | -29.279 | 67.135 | 6.918 | 1.00 | 42.67 | 6 |
| | ATOM | 530 | OG1 | THR | B | 329 | -28.799 | 65.809 | 6.686 | 1.00 | 42.52 | 8 |
| | ATOM | 531 | CG2 | THR | B | 329 | -30.702 | 67.255 | 6.375 | 1.00 | 43.52 | 6 |
| | ATOM | 532 | C | THR | B | 329 | -28.853 | 69.529 | 6.498 | 1.00 | 44.31 | 6 |

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|----|------|-----|-----|-----------|---------|--------|--------|------|-------|----|
| 5 | ATOM | 533 | O | THR B 329 | -29.432 | 69.801 | 7.535 | 1.00 | 43.72 | 8 |
| | ATOM | 534 | N | LEU B 330 | -28.589 | 70.413 | 5.546 | 1.00 | 44.62 | 7 |
| | ATOM | 535 | CA | LEU B 330 | -28.983 | 71.812 | 5.658 | 1.00 | 45.09 | 6 |
| | ATOM | 536 | CB | LEU B 330 | -28.354 | 72.608 | 4.510 | 1.00 | 44.66 | 6 |
| | ATOM | 537 | CG | LEU B 330 | -26.847 | 72.735 | 4.539 | 1.00 | 51.06 | 6 |
| 10 | ATOM | 538 | CD1 | LEU B 330 | -26.226 | 71.367 | 4.640 | 1.00 | 48.58 | 6 |
| | ATOM | 539 | CD2 | LEU B 330 | -26.364 | 73.450 | 3.299 | 1.00 | 45.18 | 6 |
| | ATOM | 540 | C | LEU B 330 | -30.508 | 71.965 | 5.652 | 1.00 | 48.06 | 6 |
| | ATOM | 541 | O | LEU B 330 | -31.211 | 71.244 | 4.959 | 1.00 | 49.33 | 8 |
| | ATOM | 542 | N | ASN B 331 | -30.988 | 72.911 | 6.458 | 1.00 | 52.20 | 7 |
| 15 | ATOM | 543 | CA | ASN B 331 | -32.407 | 73.214 | 6.588 | 1.00 | 54.41 | 6 |
| | ATOM | 544 | CB | ASN B 331 | -32.870 | 74.013 | 5.370 | 1.00 | 54.94 | 6 |
| | ATOM | 545 | CG | ASN B 331 | -33.687 | 75.220 | 5.749 | 1.00 | 60.35 | 6 |
| | ATOM | 546 | OD1 | ASN B 331 | -33.182 | 76.130 | 6.430 | 1.00 | 61.84 | 8 |
| | ATOM | 547 | ND2 | ASN B 331 | -34.935 | 75.242 | 5.324 | 1.00 | 65.92 | 7 |
| 20 | ATOM | 548 | C | ASN B 331 | -33.251 | 71.959 | 6.731 | 1.00 | 58.00 | 6 |
| | ATOM | 549 | O | ASN B 331 | -34.464 | 72.000 | 6.579 | 1.00 | 60.17 | 8 |
| | ATOM | 550 | N | GLY B 332 | -32.596 | 70.846 | 7.054 | 1.00 | 58.45 | 7 |
| | ATOM | 551 | CA | GLY B 332 | -33.295 | 69.587 | 7.235 | 1.00 | 58.55 | 6 |
| | ATOM | 552 | C | GLY B 332 | -33.909 | 69.004 | 5.984 | 1.00 | 59.79 | 6 |
| 25 | ATOM | 553 | O | GLY B 332 | -34.609 | 68.000 | 6.065 | 1.00 | 61.32 | 8 |
| | ATOM | 554 | N | GLU B 333 | -33.639 | 69.628 | 4.838 | 1.00 | 60.28 | 7 |
| | ATOM | 555 | CA | GLU B 333 | -34.196 | 69.182 | 3.571 | 1.00 | 59.13 | 6 |
| | ATOM | 556 | CB | GLU B 333 | -34.966 | 70.323 | 2.885 | 1.00 | 62.40 | 6 |
| | ATOM | 557 | CG | GLU B 333 | -36.099 | 70.963 | 3.690 | 1.00 | 75.69 | 6 |
| 30 | ATOM | 558 | CD | GLU B 333 | -36.720 | 72.135 | 2.998 | 1.00 | 80.41 | 6 |
| | ATOM | 559 | OE1 | GLU B 333 | -35.984 | 73.081 | 2.618 | 1.00 | 79.98 | 8 |
| | ATOM | 560 | OE2 | GLU B 333 | -37.966 | 72.158 | 2.830 | 1.00 | 83.81 | 8 |
| | ATOM | 561 | C | GLU B 333 | -33.110 | 68.722 | 2.624 | 1.00 | 57.18 | 6 |
| | ATOM | 562 | O | GLU B 333 | -33.236 | 67.689 | 1.974 | 1.00 | 57.50 | 8 |
| 35 | ATOM | 563 | N | MET B 334 | -32.054 | 69.528 | 2.539 | 1.00 | 55.20 | 7 |
| | ATOM | 564 | CA | MET B 334 | -30.926 | 69.259 | 1.653 | 1.00 | 50.85 | 6 |
| | ATOM | 565 | CB | MET B 334 | -30.514 | 70.563 | 0.984 | 1.00 | 48.70 | 6 |
| | ATOM | 566 | CG | MET B 334 | -29.244 | 70.460 | 0.194 | 1.00 | 45.39 | 6 |
| | ATOM | 567 | SD | MET B 334 | -28.743 | 72.008 | -0.624 | 1.00 | 44.56 | 16 |
| 40 | ATOM | 568 | CE | MET B 334 | -30.307 | 72.445 | -1.503 | 1.00 | 45.25 | 6 |
| | ATOM | 569 | C | MET B 334 | -29.711 | 68.634 | 2.319 | 1.00 | 51.59 | 6 |
| | ATOM | 570 | O | MET B 334 | -29.185 | 69.161 | 3.291 | 1.00 | 52.52 | 8 |
| | ATOM | 571 | N | ALA B 335 | -29.270 | 67.515 | 1.758 | 1.00 | 51.00 | 7 |
| | ATOM | 572 | CA | ALA B 335 | -28.106 | 66.802 | 2.267 | 1.00 | 48.98 | 6 |
| 45 | ATOM | 573 | CB | ALA B 335 | -28.377 | 65.304 | 2.274 | 1.00 | 47.86 | 6 |
| | ATOM | 574 | C | ALA B 335 | -26.931 | 67.108 | 1.371 | 1.00 | 51.01 | 6 |
| | ATOM | 575 | O | ALA B 335 | -26.936 | 66.760 | 0.190 | 1.00 | 51.61 | 8 |
| | ATOM | 576 | N | VAL B 336 | -25.921 | 67.770 | 1.930 | 1.00 | 46.62 | 7 |
| | ATOM | 577 | CA | VAL B 336 | -24.730 | 68.142 | 1.152 | 1.00 | 42.35 | 6 |
| 50 | ATOM | 578 | CB | VAL B 336 | -24.466 | 69.635 | 1.258 | 1.00 | 42.41 | 6 |
| | ATOM | 579 | CG1 | VAL B 336 | -25.695 | 70.418 | 0.860 | 1.00 | 42.00 | 6 |
| | ATOM | 580 | CG2 | VAL B 336 | -24.018 | 70.004 | 2.642 | 1.00 | 40.32 | 6 |
| | ATOM | 581 | C | VAL B 336 | -23.493 | 67.390 | 1.611 | 1.00 | 45.33 | 6 |
| | ATOM | 582 | O | VAL B 336 | -23.464 | 66.775 | 2.681 | 1.00 | 47.42 | 8 |
| 55 | ATOM | 583 | N | THR B 337 | -22.461 | 67.478 | 0.781 | 1.00 | 41.60 | 7 |
| | ATOM | 584 | CA | THR B 337 | -21.172 | 66.818 | 1.041 | 1.00 | 39.69 | 6 |
| | ATOM | 585 | CB | THR B 337 | -20.720 | 66.011 | -0.173 | 1.00 | 41.35 | 6 |
| | ATOM | 586 | OG1 | THR B 337 | -20.273 | 66.887 | -1.213 | 1.00 | 49.35 | 8 |

| | | | | | | | | | | | | |
|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 587 | CG2 | THR | B | 337 | -21.869 | 65.175 | -0.702 | 1.00 | 40.38 | 6 |
| | ATOM | 588 | C | THR | B | 337 | -20.087 | 67.846 | 1.318 | 1.00 | 37.88 | 6 |
| | ATOM | 589 | O | THR | B | 337 | -20.141 | 68.975 | 0.832 | 1.00 | 34.06 | 8 |
| | ATOM | 590 | N | ARG | B | 338 | -19.097 | 67.417 | 2.095 | 1.00 | 37.61 | 7 |
| | ATOM | 591 | CA | ARG | B | 338 | -17.942 | 68.241 | 2.442 | 1.00 | 38.68 | 6 |
| 10 | ATOM | 592 | CB | ARG | B | 338 | -16.770 | 67.333 | 2.823 | 1.00 | 35.95 | 6 |
| | ATOM | 593 | CG | ARG | B | 338 | -15.455 | 68.042 | 3.064 | 1.00 | 38.83 | 6 |
| | ATOM | 594 | CD | ARG | B | 338 | -14.348 | 67.029 | 3.319 | 1.00 | 35.88 | 6 |
| | ATOM | 595 | NE | ARG | B | 338 | -14.520 | 66.239 | 4.530 | 1.00 | 37.42 | 7 |
| | ATOM | 596 | CZ | ARG | B | 338 | -14.274 | 66.669 | 5.766 | 1.00 | 30.20 | 6 |
| 15 | ATOM | 597 | NH1 | ARG | B | 338 | -13.794 | 67.892 | 5.973 | 1.00 | 27.98 | 7 |
| | ATOM | 598 | NH2 | ARG | B | 338 | -14.481 | 65.847 | 6.788 | 1.00 | 27.40 | 7 |
| | ATOM | 599 | C | ARG | B | 338 | -17.581 | 69.075 | 1.229 | 1.00 | 38.09 | 6 |
| | ATOM | 600 | O | ARG | B | 338 | -17.537 | 70.299 | 1.284 | 1.00 | 34.12 | 8 |
| | ATOM | 601 | N | GLY | B | 339 | -17.345 | 68.383 | 0.117 | 1.00 | 41.25 | 7 |
| 20 | ATOM | 602 | CA | GLY | B | 339 | -16.981 | 69.054 | -1.119 | 1.00 | 41.35 | 6 |
| | ATOM | 603 | C | GLY | B | 339 | -18.004 | 70.109 | -1.460 | 1.00 | 41.23 | 6 |
| | ATOM | 604 | O | GLY | B | 339 | -17.736 | 71.291 | -1.330 | 1.00 | 38.30 | 8 |
| | ATOM | 605 | N | GLN | B | 340 | -19.174 | 69.665 | -1.909 | 1.00 | 38.58 | 7 |
| | ATOM | 606 | CA | GLN | B | 340 | -20.258 | 70.564 | -2.276 | 1.00 | 40.79 | 6 |
| 25 | ATOM | 607 | CB | GLN | B | 340 | -21.596 | 69.843 | -2.079 | 1.00 | 40.82 | 6 |
| | ATOM | 608 | CG | GLN | B | 340 | -21.830 | 68.657 | -3.029 | 1.00 | 41.10 | 6 |
| | ATOM | 609 | CD | GLN | B | 340 | -23.154 | 67.937 | -2.783 | 1.00 | 48.84 | 6 |
| | ATOM | 610 | OE1 | GLN | B | 340 | -23.353 | 67.313 | -1.715 | 1.00 | 50.53 | 8 |
| | ATOM | 611 | NE2 | GLN | B | 340 | -24.050 | 68.015 | -3.753 | 1.00 | 54.25 | 7 |
| 30 | ATOM | 612 | C | GLN | B | 340 | -20.239 | 71.872 | -1.475 | 1.00 | 41.50 | 6 |
| | ATOM | 613 | O | GLN | B | 340 | -20.114 | 72.958 | -2.032 | 1.00 | 42.72 | 8 |
| | ATOM | 614 | N | LEU | B | 341 | -20.352 | 71.736 | -0.156 | 1.00 | 42.00 | 7 |
| | ATOM | 615 | CA | LEU | B | 341 | -20.375 | 72.879 | 0.746 | 1.00 | 38.10 | 6 |
| | ATOM | 616 | CB | LEU | B | 341 | -20.401 | 72.419 | 2.201 | 1.00 | 36.66 | 6 |
| 35 | ATOM | 617 | CG | LEU | B | 341 | -20.678 | 73.514 | 3.194 | 1.00 | 39.94 | 6 |
| | ATOM | 618 | CD1 | LEU | B | 341 | -22.088 | 74.038 | 2.936 | 1.00 | 34.98 | 6 |
| | ATOM | 619 | CD2 | LEU | B | 341 | -20.570 | 72.990 | 4.609 | 1.00 | 40.95 | 6 |
| | ATOM | 620 | C | LEU | B | 341 | -19.170 | 73.763 | 0.543 | 1.00 | 36.37 | 6 |
| | ATOM | 621 | O | LEU | B | 341 | -19.293 | 74.974 | 0.497 | 1.00 | 37.89 | 8 |
| 40 | ATOM | 622 | N | LYS | B | 342 | -18.003 | 73.136 | 0.433 | 1.00 | 33.29 | 7 |
| | ATOM | 623 | CA | LYS | B | 342 | -16.737 | 73.843 | 0.239 | 1.00 | 35.17 | 6 |
| | ATOM | 624 | CB | LYS | B | 342 | -15.603 | 72.821 | 0.176 | 1.00 | 34.97 | 6 |
| | ATOM | 625 | CG | LYS | B | 342 | -14.210 | 73.401 | 0.306 | 1.00 | 40.00 | 6 |
| | ATOM | 626 | CD | LYS | B | 342 | -13.155 | 72.288 | 0.316 | 1.00 | 34.48 | 6 |
| 45 | ATOM | 627 | CE | LYS | B | 342 | -11.775 | 72.809 | 0.755 | 1.00 | 37.54 | 6 |
| | ATOM | 628 | NZ | LYS | B | 342 | -10.790 | 71.680 | 0.981 | 1.00 | 42.32 | 7 |
| | ATOM | 629 | C | LYS | B | 342 | -16.744 | 74.685 | -1.038 | 1.00 | 38.29 | 6 |
| | ATOM | 630 | O | LYS | B | 342 | -16.725 | 75.911 | -0.993 | 1.00 | 36.23 | 8 |
| | ATOM | 631 | N | ASN | B | 343 | -16.760 | 73.990 | -2.172 | 1.00 | 39.25 | 7 |
| 50 | ATOM | 632 | CA | ASN | B | 343 | -16.762 | 74.609 | -3.481 | 1.00 | 40.19 | 6 |
| | ATOM | 633 | CB | ASN | B | 343 | -16.977 | 73.539 | -4.551 | 1.00 | 37.96 | 6 |
| | ATOM | 634 | CG | ASN | B | 343 | -16.178 | 72.272 | -4.277 | 1.00 | 39.22 | 6 |
| | ATOM | 635 | OD1 | ASN | B | 343 | -14.938 | 72.313 | -4.106 | 1.00 | 42.37 | 8 |
| | ATOM | 636 | ND2 | ASN | B | 343 | -16.877 | 71.144 | -4.259 | 1.00 | 42.19 | 7 |
| 55 | ATOM | 637 | C | ASN | B | 343 | -17.894 | 75.624 | -3.547 | 1.00 | 40.12 | 6 |
| | ATOM | 638 | O | ASN | B | 343 | -17.835 | 76.600 | -4.284 | 1.00 | 36.01 | 8 |
| | ATOM | 639 | N | GLY | B | 344 | -18.934 | 75.361 | -2.756 | 1.00 | 40.95 | 7 |
| | ATOM | 640 | CA | GLY | B | 344 | -20.101 | 76.222 | -2.709 | 1.00 | 39.25 | 6 |

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|----|------|-----|-----|-----------|---------|--------|--------|------|-------|---|
| 5 | ATOM | 641 | C | GLY B 344 | -19.867 | 77.636 | -2.258 | 1.00 | 38.26 | 6 |
| | ATOM | 642 | O | GLY B 344 | -20.715 | 78.501 | -2.484 | 1.00 | 35.69 | 8 |
| | ATOM | 643 | N | GLY B 345 | -18.724 | 77.871 | -1.619 | 1.00 | 35.89 | 7 |
| | ATOM | 644 | CA | GLY B 345 | -18.426 | 79.209 | -1.159 | 1.00 | 34.00 | 6 |
| | ATOM | 645 | C | GLY B 345 | -17.848 | 79.298 | 0.230 | 1.00 | 38.64 | 6 |
| 10 | ATOM | 646 | O | GLY B 345 | -17.216 | 80.303 | 0.573 | 1.00 | 38.14 | 8 |
| | ATOM | 647 | N | LEU B 346 | -18.071 | 78.266 | 1.041 | 1.00 | 39.52 | 7 |
| | ATOM | 648 | CA | LEU B 346 | -17.563 | 78.279 | 2.403 | 1.00 | 36.05 | 6 |
| | ATOM | 649 | CB | LEU B 346 | -18.311 | 77.256 | 3.269 | 1.00 | 35.72 | 6 |
| | ATOM | 650 | CG | LEU B 346 | -19.800 | 77.473 | 3.378 | 1.00 | 34.89 | 6 |
| 15 | ATOM | 651 | CD1 | LEU B 346 | -20.322 | 76.678 | 4.554 | 1.00 | 44.09 | 6 |
| | ATOM | 652 | CD2 | LEU B 346 | -20.086 | 78.937 | 3.612 | 1.00 | 34.84 | 6 |
| | ATOM | 653 | C | LEU B 346 | -16.079 | 78.018 | 2.445 | 1.00 | 33.52 | 6 |
| | ATOM | 654 | O | LEU B 346 | -15.392 | 78.387 | 3.394 | 1.00 | 35.58 | 8 |
| | ATOM | 655 | N | GLY B 347 | -15.586 | 77.388 | 1.385 | 1.00 | 30.47 | 7 |
| 20 | ATOM | 656 | CA | GLY B 347 | -14.174 | 77.078 | 1.305 | 1.00 | 33.01 | 6 |
| | ATOM | 657 | C | GLY B 347 | -13.768 | 76.214 | 2.477 | 1.00 | 30.72 | 6 |
| | ATOM | 658 | O | GLY B 347 | -14.433 | 75.243 | 2.808 | 1.00 | 30.89 | 8 |
| | ATOM | 659 | N | VAL B 348 | -12.647 | 76.585 | 3.087 | 1.00 | 31.30 | 7 |
| | ATOM | 660 | CA | VAL B 348 | -12.097 | 75.867 | 4.227 | 1.00 | 31.27 | 6 |
| 25 | ATOM | 661 | CB | VAL B 348 | -10.889 | 76.609 | 4.817 | 1.00 | 31.66 | 6 |
| | ATOM | 662 | CG1 | VAL B 348 | -11.292 | 77.974 | 5.360 | 1.00 | 20.19 | 6 |
| | ATOM | 663 | CG2 | VAL B 348 | -10.250 | 75.786 | 5.905 | 1.00 | 24.77 | 6 |
| | ATOM | 664 | C | VAL B 348 | -13.136 | 75.651 | 5.360 | 1.00 | 33.84 | 6 |
| | ATOM | 665 | O | VAL B 348 | -13.002 | 74.707 | 6.153 | 1.00 | 29.99 | 8 |
| 30 | ATOM | 666 | N | VAL B 349 | -14.157 | 76.518 | 5.449 | 1.00 | 33.31 | 7 |
| | ATOM | 667 | CA | VAL B 349 | -15.147 | 76.339 | 6.483 | 1.00 | 32.23 | 6 |
| | ATOM | 668 | CB | VAL B 349 | -16.226 | 77.393 | 6.476 | 1.00 | 32.59 | 6 |
| | ATOM | 669 | CG1 | VAL B 349 | -17.342 | 76.979 | 7.399 | 1.00 | 33.68 | 6 |
| | ATOM | 670 | CG2 | VAL B 349 | -15.667 | 78.703 | 6.959 | 1.00 | 32.30 | 6 |
| 35 | ATOM | 671 | C | VAL B 349 | -15.792 | 74.987 | 6.380 | 1.00 | 34.91 | 6 |
| | ATOM | 672 | O | VAL B 349 | -16.055 | 74.359 | 7.394 | 1.00 | 33.73 | 8 |
| | ATOM | 673 | N | SER B 350 | -16.054 | 74.507 | 5.176 | 1.00 | 32.81 | 7 |
| | ATOM | 674 | CA | SER B 350 | -16.695 | 73.215 | 5.100 | 1.00 | 30.10 | 6 |
| | ATOM | 675 | CB | SER B 350 | -16.772 | 72.697 | 3.684 | 1.00 | 24.95 | 6 |
| 40 | ATOM | 676 | OG | SER B 350 | -17.538 | 71.502 | 3.644 | 1.00 | 23.16 | 8 |
| | ATOM | 677 | C | SER B 350 | -15.910 | 72.254 | 5.942 | 1.00 | 31.59 | 6 |
| | ATOM | 678 | O | SER B 350 | -16.417 | 71.807 | 6.950 | 1.00 | 37.62 | 8 |
| | ATOM | 679 | N | ASP B 351 | -14.675 | 71.942 | 5.565 | 1.00 | 28.60 | 7 |
| | ATOM | 680 | CA | ASP B 351 | -13.905 | 71.010 | 6.378 | 1.00 | 29.82 | 6 |
| 45 | ATOM | 681 | CB | ASP B 351 | -12.419 | 71.139 | 6.050 | 1.00 | 27.49 | 6 |
| | ATOM | 682 | CG | ASP B 351 | -12.151 | 71.094 | 4.585 | 1.00 | 30.22 | 6 |
| | ATOM | 683 | OD1 | ASP B 351 | -12.013 | 72.174 | 3.954 | 1.00 | 32.61 | 8 |
| | ATOM | 684 | OD2 | ASP B 351 | -12.064 | 69.980 | 4.017 | 1.00 | 30.02 | 8 |
| | ATOM | 685 | C | ASP B 351 | -14.176 | 71.343 | 7.861 | 1.00 | 30.63 | 6 |
| 50 | ATOM | 686 | O | ASP B 351 | -14.458 | 70.474 | 8.681 | 1.00 | 29.54 | 8 |
| | ATOM | 687 | N | ALA B 352 | -14.111 | 72.629 | 8.177 | 1.00 | 25.33 | 7 |
| | ATOM | 688 | CA | ALA B 352 | -14.346 | 73.092 | 9.533 | 1.00 | 28.59 | 6 |
| | ATOM | 689 | CB | ALA B 352 | -14.252 | 74.606 | 9.572 | 1.00 | 20.95 | 6 |
| | ATOM | 690 | C | ALA B 352 | -15.690 | 72.630 | 10.086 | 1.00 | 29.69 | 6 |
| 55 | ATOM | 691 | O | ALA B 352 | -15.757 | 72.068 | 11.164 | 1.00 | 30.36 | 8 |
| | ATOM | 692 | N | ILE B 353 | -16.754 | 72.884 | 9.330 | 1.00 | 27.63 | 7 |
| | ATOM | 693 | CA | ILE B 353 | -18.096 | 72.506 | 9.729 | 1.00 | 27.55 | 6 |
| | ATOM | 694 | CB | ILE B 353 | -19.144 | 73.129 | 8.800 | 1.00 | 28.04 | 6 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 695 | CG2 | ILE | B | 353 | -20.529 | 72.673 | 9.195 | 1.00 | 23.68 | 6 |
| | ATOM | 696 | CG1 | ILE | B | 353 | -19.108 | 74.657 | 8.869 | 1.00 | 27.33 | 6 |
| | ATOM | 697 | CD1 | ILE | B | 353 | -20.141 | 75.313 | 7.964 | 1.00 | 26.23 | 6 |
| | ATOM | 698 | C | ILE | B | 353 | -18.309 | 71.002 | 9.775 | 1.00 | 30.88 | 6 |
| | ATOM | 699 | O | ILE | B | 353 | -19.021 | 70.499 | 10.639 | 1.00 | 31.22 | 8 |
| 10 | ATOM | 700 | N | PHE | B | 354 | -17.728 | 70.279 | 8.822 | 1.00 | 29.86 | 7 |
| | ATOM | 701 | CA | PHE | B | 354 | -17.881 | 68.831 | 8.797 | 1.00 | 31.08 | 6 |
| | ATOM | 702 | CB | PHE | B | 354 | -17.461 | 68.249 | 7.439 | 1.00 | 28.80 | 6 |
| | ATOM | 703 | CG | PHE | B | 354 | -18.568 | 68.233 | 6.405 | 1.00 | 28.80 | 6 |
| | ATOM | 704 | CD1 | PHE | B | 354 | -19.031 | 69.403 | 5.833 | 1.00 | 30.96 | 6 |
| 15 | ATOM | 705 | CD2 | PHE | B | 354 | -19.150 | 67.027 | 6.034 | 1.00 | 29.45 | 6 |
| | ATOM | 706 | CE1 | PHE | B | 354 | -20.066 | 69.362 | 4.902 | 1.00 | 27.12 | 6 |
| | ATOM | 707 | CE2 | PHE | B | 354 | -20.186 | 66.978 | 5.104 | 1.00 | 25.19 | 6 |
| | ATOM | 708 | CZ | PHE | B | 354 | -20.644 | 68.146 | 4.535 | 1.00 | 28.09 | 6 |
| | ATOM | 709 | C | PHE | B | 354 | -17.041 | 68.223 | 9.913 | 1.00 | 29.17 | 6 |
| 20 | ATOM | 710 | O | PHE | B | 354 | -17.544 | 67.429 | 10.700 | 1.00 | 32.62 | 8 |
| | ATOM | 711 | N | ASP | B | 355 | -15.761 | 68.593 | 9.972 | 1.00 | 23.86 | 7 |
| | ATOM | 712 | CA | ASP | B | 355 | -14.864 | 68.090 | 11.005 | 1.00 | 25.34 | 6 |
| | ATOM | 713 | CB | ASP | B | 355 | -13.582 | 68.929 | 11.045 | 1.00 | 21.41 | 6 |
| | ATOM | 714 | CG | ASP | B | 355 | -12.548 | 68.456 | 10.086 | 1.00 | 32.08 | 6 |
| 25 | ATOM | 715 | OD1 | ASP | B | 355 | -12.899 | 68.069 | 8.944 | 1.00 | 33.58 | 8 |
| | ATOM | 716 | OD2 | ASP | B | 355 | -11.345 | 68.477 | 10.450 | 1.00 | 33.20 | 8 |
| | ATOM | 717 | C | ASP | B | 355 | -15.570 | 68.153 | 12.357 | 1.00 | 27.86 | 6 |
| | ATOM | 718 | O | ASP | B | 355 | -15.430 | 67.257 | 13.182 | 1.00 | 32.42 | 8 |
| | ATOM | 719 | N | LEU | B | 356 | -16.339 | 69.223 | 12.561 | 1.00 | 26.84 | 7 |
| 30 | ATOM | 720 | CA | LEU | B | 356 | -17.085 | 69.400 | 13.803 | 1.00 | 28.66 | 6 |
| | ATOM | 721 | CB | LEU | B | 356 | -17.832 | 70.742 | 13.800 | 1.00 | 25.37 | 6 |
| | ATOM | 722 | CG | LEU | B | 356 | -18.655 | 71.091 | 15.023 | 1.00 | 27.61 | 6 |
| | ATOM | 723 | CD1 | LEU | B | 356 | -17.729 | 71.248 | 16.191 | 1.00 | 25.43 | 6 |
| | ATOM | 724 | CD2 | LEU | B | 356 | -19.430 | 72.363 | 14.808 | 1.00 | 27.49 | 6 |
| 35 | ATOM | 725 | C | LEU | B | 356 | -18.084 | 68.260 | 13.883 | 1.00 | 30.44 | 6 |
| | ATOM | 726 | O | LEU | B | 356 | -18.054 | 67.445 | 14.804 | 1.00 | 31.55 | 8 |
| | ATOM | 727 | N | GLY | B | 357 | -18.972 | 68.214 | 12.891 | 1.00 | 32.69 | 7 |
| | ATOM | 728 | CA | GLY | B | 357 | -20.001 | 67.186 | 12.846 | 1.00 | 29.87 | 6 |
| | ATOM | 729 | C | GLY | B | 357 | -19.486 | 65.832 | 13.279 | 1.00 | 33.12 | 6 |
| 40 | ATOM | 730 | O | GLY | B | 357 | -20.032 | 65.246 | 14.207 | 1.00 | 29.41 | 8 |
| | ATOM | 731 | N | MET | B | 358 | -18.444 | 65.351 | 12.593 | 1.00 | 33.31 | 7 |
| | ATOM | 732 | CA | MET | B | 358 | -17.834 | 64.066 | 12.902 | 1.00 | 35.87 | 6 |
| | ATOM | 733 | CB | MET | B | 358 | -16.513 | 63.903 | 12.151 | 1.00 | 34.56 | 6 |
| | ATOM | 734 | CG | MET | B | 358 | -16.649 | 63.908 | 10.657 | 1.00 | 46.43 | 6 |
| 45 | ATOM | 735 | SD | MET | B | 358 | -15.094 | 63.597 | 9.751 | 1.00 | 42.13 | 16 |
| | ATOM | 736 | CE | MET | B | 358 | -14.121 | 65.063 | 10.228 | 1.00 | 44.29 | 6 |
| | ATOM | 737 | C | MET | B | 358 | -17.552 | 63.976 | 14.392 | 1.00 | 33.26 | 6 |
| | ATOM | 738 | O | MET | B | 358 | -18.019 | 63.075 | 15.075 | 1.00 | 36.39 | 8 |
| | ATOM | 739 | N | SER | B | 359 | -16.766 | 64.933 | 14.875 | 1.00 | 33.31 | 7 |
| 50 | ATOM | 740 | CA | SER | B | 359 | -16.380 | 64.998 | 16.270 | 1.00 | 34.39 | 6 |
| | ATOM | 741 | CB | SER | B | 359 | -15.724 | 66.339 | 16.541 | 1.00 | 30.84 | 6 |
| | ATOM | 742 | OG | SER | B | 359 | -15.130 | 66.355 | 17.825 | 1.00 | 47.14 | 8 |
| | ATOM | 743 | C | SER | B | 359 | -17.579 | 64.813 | 17.169 | 1.00 | 36.43 | 6 |
| | ATOM | 744 | O | SER | B | 359 | -17.635 | 63.853 | 17.922 | 1.00 | 35.46 | 8 |
| 55 | ATOM | 745 | N | LEU | B | 360 | -18.525 | 65.744 | 17.079 | 1.00 | 36.74 | 7 |
| | ATOM | 746 | CA | LEU | B | 360 | -19.741 | 65.729 | 17.889 | 1.00 | 35.44 | 6 |
| | ATOM | 747 | CB | LEU | B | 360 | -20.706 | 66.817 | 17.405 | 1.00 | 34.16 | 6 |
| | ATOM | 748 | CG | LEU | B | 360 | -20.263 | 68.255 | 17.575 | 1.00 | 34.59 | 6 |

| | | | | | | | | | | |
|----|------|-----|-----|-----------|---------|--------|--------|------|-------|---|
| 5 | ATOM | 749 | CD1 | LEU B 360 | -21.394 | 69.181 | 17.212 | 1.00 | 33.53 | 6 |
| | ATOM | 750 | CD2 | LEU B 360 | -19.869 | 68.486 | 19.010 | 1.00 | 31.69 | 6 |
| | ATOM | 751 | C | LEU B 360 | -20.464 | 64.397 | 17.924 | 1.00 | 38.72 | 6 |
| | ATOM | 752 | O | LEU B 360 | -21.021 | 64.011 | 18.958 | 1.00 | 38.29 | 8 |
| | ATOM | 753 | N | SER B 361 | -20.466 | 63.708 | 16.791 | 1.00 | 40.96 | 7 |
| 10 | ATOM | 754 | CA | SER B 361 | -21.106 | 62.416 | 16.721 | 1.00 | 45.67 | 6 |
| | ATOM | 755 | CB | SER B 361 | -20.532 | 61.630 | 15.551 | 1.00 | 46.45 | 6 |
| | ATOM | 756 | OG | SER B 361 | -20.750 | 62.314 | 14.322 | 1.00 | 51.81 | 8 |
| | ATOM | 757 | C | SER B 361 | -20.895 | 61.638 | 18.018 | 1.00 | 44.49 | 6 |
| | ATOM | 758 | O | SER B 361 | -21.696 | 60.793 | 18.362 | 1.00 | 46.67 | 8 |
| 15 | ATOM | 759 | N | SER B 362 | -19.811 | 61.953 | 18.726 | 1.00 | 41.44 | 7 |
| | ATOM | 760 | CA | SER B 362 | -19.453 | 61.309 | 19.972 | 1.00 | 42.13 | 6 |
| | ATOM | 761 | CB | SER B 362 | -17.962 | 61.510 | 20.234 | 1.00 | 42.61 | 6 |
| | ATOM | 762 | OG | SER B 362 | -17.164 | 61.025 | 19.158 | 1.00 | 51.87 | 8 |
| | ATOM | 763 | C | SER B 362 | -20.228 | 61.812 | 21.174 | 1.00 | 38.41 | 6 |
| 20 | ATOM | 764 | O | SER B 362 | -20.602 | 61.025 | 22.035 | 1.00 | 38.01 | 8 |
| | ATOM | 765 | N | PHE B 363 | -20.455 | 63.123 | 21.228 | 1.00 | 34.55 | 7 |
| | ATOM | 766 | CA | PHE B 363 | -21.150 | 63.735 | 22.346 | 1.00 | 32.96 | 6 |
| | ATOM | 767 | CB | PHE B 363 | -21.006 | 65.245 | 22.285 | 1.00 | 31.99 | 6 |
| | ATOM | 768 | CG | PHE B 363 | -19.578 | 65.719 | 22.378 | 1.00 | 29.97 | 6 |
| 25 | ATOM | 769 | CD1 | PHE B 363 | -19.286 | 67.058 | 22.447 | 1.00 | 30.61 | 6 |
| | ATOM | 770 | CD2 | PHE B 363 | -18.536 | 64.800 | 22.391 | 1.00 | 32.02 | 6 |
| | ATOM | 771 | CE1 | PHE B 363 | -17.966 | 67.489 | 22.543 | 1.00 | 33.67 | 6 |
| | ATOM | 772 | CE2 | PHE B 363 | -17.221 | 65.222 | 22.484 | 1.00 | 30.91 | 6 |
| | ATOM | 773 | CZ | PHE B 363 | -16.927 | 66.557 | 22.554 | 1.00 | 29.33 | 6 |
| 30 | ATOM | 774 | C | PHE B 363 | -22.617 | 63.361 | 22.482 | 1.00 | 30.52 | 6 |
| | ATOM | 775 | O | PHE B 363 | -23.142 | 63.331 | 23.596 | 1.00 | 32.19 | 8 |
| | ATOM | 776 | N | ASN B 364 | -23.279 | 63.075 | 21.361 | 1.00 | 33.51 | 7 |
| | ATOM | 777 | CA | ASN B 364 | -24.683 | 62.701 | 21.377 | 1.00 | 38.03 | 6 |
| | ATOM | 778 | CB | ASN B 364 | -24.855 | 61.369 | 22.111 | 1.00 | 42.32 | 6 |
| 35 | ATOM | 779 | CG | ASN B 364 | -24.008 | 60.271 | 21.524 | 1.00 | 53.11 | 6 |
| | ATOM | 780 | OD1 | ASN B 364 | -24.183 | 59.895 | 20.344 | 1.00 | 59.51 | 8 |
| | ATOM | 781 | ND2 | ASN B 364 | -23.102 | 59.746 | 22.325 | 1.00 | 55.95 | 7 |
| | ATOM | 782 | C | ASN B 364 | -25.494 | 63.771 | 22.091 | 1.00 | 31.89 | 6 |
| | ATOM | 783 | O | ASN B 364 | -26.279 | 63.471 | 22.990 | 1.00 | 30.28 | 8 |
| 40 | ATOM | 784 | N | LEU B 365 | -25.306 | 65.018 | 21.673 | 1.00 | 27.62 | 7 |
| | ATOM | 785 | CA | LEU B 365 | -26.005 | 66.144 | 22.280 | 1.00 | 29.36 | 6 |
| | ATOM | 786 | CB | LEU B 365 | -25.402 | 67.443 | 21.743 | 1.00 | 27.54 | 6 |
| | ATOM | 787 | CG | LEU B 365 | -23.897 | 67.453 | 21.738 | 1.00 | 38.91 | 6 |
| | ATOM | 788 | CD1 | LEU B 365 | -23.391 | 68.766 | 21.190 | 1.00 | 34.47 | 6 |
| 45 | ATOM | 789 | CD2 | LEU B 365 | -23.393 | 67.214 | 23.143 | 1.00 | 34.24 | 6 |
| | ATOM | 790 | C | LEU B 365 | -27.496 | 66.074 | 21.987 | 1.00 | 26.23 | 6 |
| | ATOM | 791 | O | LEU B 365 | -27.911 | 65.790 | 20.863 | 1.00 | 27.06 | 8 |
| | ATOM | 792 | N | ASP B 366 | -28.296 | 66.321 | 23.022 | 1.00 | 25.23 | 7 |
| | ATOM | 793 | CA | ASP B 366 | -29.752 | 66.320 | 22.878 | 1.00 | 26.07 | 6 |
| 50 | ATOM | 794 | CB | ASP B 366 | -30.441 | 65.651 | 24.076 | 1.00 | 29.68 | 6 |
| | ATOM | 795 | CG | ASP B 366 | -30.221 | 66.374 | 25.360 | 1.00 | 35.74 | 6 |
| | ATOM | 796 | OD1 | ASP B 366 | -30.277 | 67.617 | 25.387 | 1.00 | 36.78 | 8 |
| | ATOM | 797 | OD2 | ASP B 366 | -30.017 | 65.711 | 26.410 | 1.00 | 41.23 | 8 |
| | ATOM | 798 | C | ASP B 366 | -30.230 | 67.752 | 22.740 | 1.00 | 27.70 | 6 |
| 55 | ATOM | 799 | O | ASP B 366 | -29.552 | 68.678 | 23.171 | 1.00 | 31.94 | 8 |
| | ATOM | 800 | N | ASP B 367 | -31.409 | 67.913 | 22.142 | 1.00 | 29.18 | 7 |
| | ATOM | 801 | CA | ASP B 367 | -32.031 | 69.225 | 21.930 | 1.00 | 32.72 | 6 |
| | ATOM | 802 | CB | ASP B 367 | -33.558 | 69.106 | 22.071 | 1.00 | 38.04 | 6 |

SUBSTITUTE SHEET (RULE 26)

| | | | | | | | | | | | | |
|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 803 | CG | ASP | B | 367 | -34.172 | 68.166 | 21.081 | 1.00 | 42.43 | 6 |
| | ATOM | 804 | OD1 | ASP | B | 367 | -34.051 | 68.373 | 19.854 | 1.00 | 35.95 | 8 |
| | ATOM | 805 | OD2 | ASP | B | 367 | -34.829 | 67.188 | 21.504 | 1.00 | 51.42 | 8 |
| | ATOM | 806 | C | ASP | B | 367 | -31.496 | 70.238 | 22.959 | 1.00 | 33.71 | 6 |
| | ATOM | 807 | O | ASP | B | 367 | -30.791 | 71.188 | 22.624 | 1.00 | 38.30 | 8 |
| 10 | ATOM | 808 | N | THR | B | 368 | -31.858 | 69.997 | 24.218 | 1.00 | 31.06 | 7 |
| | ATOM | 809 | CA | THR | B | 368 | -31.453 | 70.822 | 25.344 | 1.00 | 26.28 | 6 |
| | ATOM | 810 | CB | THR | B | 368 | -31.567 | 70.020 | 26.643 | 1.00 | 27.30 | 6 |
| | ATOM | 811 | OG1 | THR | B | 368 | -32.916 | 69.578 | 26.824 | 1.00 | 33.42 | 8 |
| | ATOM | 812 | CG2 | THR | B | 368 | -31.143 | 70.855 | 27.824 | 1.00 | 25.16 | 6 |
| 15 | ATOM | 813 | C | THR | B | 368 | -30.025 | 71.315 | 25.181 | 1.00 | 21.13 | 6 |
| | ATOM | 814 | O | THR | B | 368 | -29.746 | 72.508 | 25.150 | 1.00 | 23.17 | 8 |
| | ATOM | 815 | N | GLU | B | 369 | -29.123 | 70.354 | 25.072 | 1.00 | 21.32 | 7 |
| | ATOM | 816 | CA | GLU | B | 369 | -27.711 | 70.634 | 24.932 | 1.00 | 28.00 | 6 |
| | ATOM | 817 | CB | GLU | B | 369 | -26.947 | 69.306 | 24.878 | 1.00 | 32.79 | 6 |
| 20 | ATOM | 818 | CG | GLU | B | 369 | -27.229 | 68.433 | 26.130 | 1.00 | 36.29 | 6 |
| | ATOM | 819 | CD | GLU | B | 369 | -26.689 | 67.051 | 26.083 | 1.00 | 41.03 | 6 |
| | ATOM | 820 | OE1 | GLU | B | 369 | -26.960 | 66.318 | 25.102 | 1.00 | 42.05 | 8 |
| | ATOM | 821 | OE2 | GLU | B | 369 | -25.992 | 66.645 | 27.048 | 1.00 | 42.03 | 8 |
| | ATOM | 822 | C | GLU | B | 369 | -27.428 | 71.527 | 23.731 | 1.00 | 25.57 | 6 |
| 25 | ATOM | 823 | O | GLU | B | 369 | -26.780 | 72.549 | 23.886 | 1.00 | 20.56 | 8 |
| | ATOM | 824 | N | VAL | B | 370 | -27.922 | 71.154 | 22.548 | 1.00 | 25.39 | 7 |
| | ATOM | 825 | CA | VAL | B | 370 | -27.710 | 71.968 | 21.355 | 1.00 | 25.99 | 6 |
| | ATOM | 826 | CB | VAL | B | 370 | -28.457 | 71.429 | 20.130 | 1.00 | 26.15 | 6 |
| | ATOM | 827 | CG1 | VAL | B | 370 | -28.255 | 72.358 | 18.953 | 1.00 | 27.65 | 6 |
| 30 | ATOM | 828 | CG2 | VAL | B | 370 | -28.014 | 70.021 | 19.788 | 1.00 | 17.70 | 6 |
| | ATOM | 829 | C | VAL | B | 370 | -28.238 | 73.346 | 21.676 | 1.00 | 26.49 | 6 |
| | ATOM | 830 | O | VAL | B | 370 | -27.580 | 74.351 | 21.445 | 1.00 | 28.16 | 8 |
| | ATOM | 831 | N | ALA | B | 371 | -29.450 | 73.362 | 22.213 | 1.00 | 21.01 | 7 |
| | ATOM | 832 | CA | ALA | B | 371 | -30.145 | 74.589 | 22.573 | 1.00 | 19.57 | 6 |
| 35 | ATOM | 833 | CB | ALA | B | 371 | -31.414 | 74.246 | 23.335 | 1.00 | 18.62 | 6 |
| | ATOM | 834 | C | ALA | B | 371 | -29.256 | 75.501 | 23.401 | 1.00 | 23.48 | 6 |
| | ATOM | 835 | O | ALA | B | 371 | -28.936 | 76.613 | 22.989 | 1.00 | 32.67 | 8 |
| | ATOM | 836 | N | LEU | B | 372 | -28.860 | 75.008 | 24.571 | 1.00 | 22.89 | 7 |
| | ATOM | 837 | CA | LEU | B | 372 | -27.999 | 75.758 | 25.472 | 1.00 | 23.28 | 6 |
| 40 | ATOM | 838 | CB | LEU | B | 372 | -27.606 | 74.860 | 26.658 | 1.00 | 27.76 | 6 |
| | ATOM | 839 | CG | LEU | B | 372 | -28.728 | 74.524 | 27.619 | 1.00 | 21.18 | 6 |
| | ATOM | 840 | CD1 | LEU | B | 372 | -28.272 | 73.529 | 28.648 | 1.00 | 27.64 | 6 |
| | ATOM | 841 | CD2 | LEU | B | 372 | -29.198 | 75.801 | 28.284 | 1.00 | 20.90 | 6 |
| | ATOM | 842 | C | LEU | B | 372 | -26.769 | 76.268 | 24.722 | 1.00 | 21.34 | 6 |
| 45 | ATOM | 843 | O | LEU | B | 372 | -26.439 | 77.454 | 24.762 | 1.00 | 23.16 | 8 |
| | ATOM | 844 | N | LEU | B | 373 | -26.111 | 75.349 | 24.023 | 1.00 | 24.42 | 7 |
| | ATOM | 845 | CA | LEU | B | 373 | -24.916 | 75.669 | 23.254 | 1.00 | 23.78 | 6 |
| | ATOM | 846 | CB | LEU | B | 373 | -24.525 | 74.446 | 22.396 | 1.00 | 22.18 | 6 |
| | ATOM | 847 | CG | LEU | B | 373 | -23.098 | 74.283 | 21.942 | 1.00 | 31.52 | 6 |
| 50 | ATOM | 848 | CD1 | LEU | B | 373 | -22.196 | 74.576 | 23.100 | 1.00 | 31.93 | 6 |
| | ATOM | 849 | CD2 | LEU | B | 373 | -22.873 | 72.889 | 21.457 | 1.00 | 30.24 | 6 |
| | ATOM | 850 | C | LEU | B | 373 | -25.235 | 76.902 | 22.405 | 1.00 | 25.69 | 6 |
| | ATOM | 851 | O | LEU | B | 373 | -24.491 | 77.880 | 22.416 | 1.00 | 30.13 | 8 |
| | ATOM | 852 | N | GLN | B | 374 | -26.368 | 76.842 | 21.707 | 1.00 | 26.24 | 7 |
| 55 | ATOM | 853 | CA | GLN | B | 374 | -26.836 | 77.922 | 20.839 | 1.00 | 21.60 | 6 |
| | ATOM | 854 | CB | GLN | B | 374 | -28.196 | 77.571 | 20.221 | 1.00 | 24.57 | 6 |
| | ATOM | 855 | CG | GLN | B | 374 | -28.188 | 76.330 | 19.348 | 1.00 | 21.02 | 6 |
| | ATOM | 856 | CD | GLN | B | 374 | -29.538 | 76.071 | 18.698 | 1.00 | 22.86 | 6 |

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|----|------|-----|-----|-----------|---------|--------|--------|------|-------|----|
| 5 | ATOM | 857 | OE1 | GLN B 374 | -29.720 | 75.049 | 18.009 | 1.00 | 24.07 | 8 |
| | ATOM | 858 | NE2 | GLN B 374 | -30.473 | 76.980 | 18.901 | 1.00 | 25.59 | 7 |
| | ATOM | 859 | C | GLN B 374 | -26.988 | 79.249 | 21.569 | 1.00 | 20.66 | 6 |
| | ATOM | 860 | O | GLN B 374 | -26.733 | 80.307 | 20.994 | 1.00 | 24.47 | 8 |
| | ATOM | 861 | N | ALA B 375 | -27.429 | 79.182 | 22.825 | 1.00 | 16.26 | 7 |
| 10 | ATOM | 862 | CA | ALA B 375 | -27.639 | 80.374 | 23.631 | 1.00 | 17.16 | 6 |
| | ATOM | 863 | CB | ALA B 375 | -28.435 | 80.025 | 24.865 | 1.00 | 19.53 | 6 |
| | ATOM | 864 | C | ALA B 375 | -26.304 | 80.966 | 24.025 | 1.00 | 25.13 | 6 |
| | ATOM | 865 | O | ALA B 375 | -26.074 | 82.154 | 23.833 | 1.00 | 23.81 | 8 |
| | ATOM | 866 | N | VAL B 376 | -25.433 | 80.111 | 24.568 | 1.00 | 24.57 | 7 |
| 15 | ATOM | 867 | CA | VAL B 376 | -24.102 | 80.526 | 24.986 | 1.00 | 25.80 | 6 |
| | ATOM | 868 | CB | VAL B 376 | -23.192 | 79.321 | 25.234 | 1.00 | 26.48 | 6 |
| | ATOM | 869 | CG1 | VAL B 376 | -21.806 | 79.780 | 25.620 | 1.00 | 23.20 | 6 |
| | ATOM | 870 | CG2 | VAL B 376 | -23.771 | 78.433 | 26.310 | 1.00 | 19.08 | 6 |
| | ATOM | 871 | C | VAL B 376 | -23.510 | 81.403 | 23.898 | 1.00 | 25.69 | 6 |
| 20 | ATOM | 872 | O | VAL B 376 | -22.796 | 82.364 | 24.166 | 1.00 | 27.87 | 8 |
| | ATOM | 873 | N | LEU B 377 | -23.827 | 81.049 | 22.659 | 1.00 | 23.09 | 7 |
| | ATOM | 874 | CA | LEU B 377 | -23.340 | 81.774 | 21.492 | 1.00 | 22.86 | 6 |
| | ATOM | 875 | CB | LEU B 377 | -23.552 | 80.920 | 20.230 | 1.00 | 18.50 | 6 |
| | ATOM | 876 | CG | LEU B 377 | -22.756 | 79.638 | 20.146 | 1.00 | 22.65 | 6 |
| 25 | ATOM | 877 | CD1 | LEU B 377 | -23.221 | 78.786 | 19.000 | 1.00 | 16.70 | 6 |
| | ATOM | 878 | CD2 | LEU B 377 | -21.300 | 79.995 | 20.000 | 1.00 | 19.58 | 6 |
| | ATOM | 879 | C | LEU B 377 | -24.073 | 83.102 | 21.384 | 1.00 | 26.14 | 6 |
| | ATOM | 880 | O | LEU B 377 | -23.464 | 84.164 | 21.419 | 1.00 | 20.62 | 8 |
| | ATOM | 881 | N | LEU B 378 | -25.396 | 83.023 | 21.265 | 1.00 | 28.99 | 7 |
| 30 | ATOM | 882 | CA | LEU B 378 | -26.228 | 84.217 | 21.147 | 1.00 | 28.87 | 6 |
| | ATOM | 883 | CB | LEU B 378 | -27.696 | 83.894 | 21.450 | 1.00 | 26.89 | 6 |
| | ATOM | 884 | CG | LEU B 378 | -28.648 | 85.068 | 21.500 | 1.00 | 28.83 | 6 |
| | ATOM | 885 | CD1 | LEU B 378 | -28.507 | 85.854 | 20.225 | 1.00 | 27.97 | 6 |
| | ATOM | 886 | CD2 | LEU B 378 | -30.072 | 84.605 | 21.692 | 1.00 | 27.69 | 6 |
| 35 | ATOM | 887 | C | LEU B 378 | -25.738 | 85.280 | 22.090 | 1.00 | 31.09 | 6 |
| | ATOM | 888 | O | LEU B 378 | -25.398 | 86.379 | 21.651 | 1.00 | 31.77 | 8 |
| | ATOM | 889 | N | MET B 379 | -25.695 | 84.931 | 23.376 | 1.00 | 31.44 | 7 |
| | ATOM | 890 | CA | MET B 379 | -25.291 | 85.851 | 24.434 | 1.00 | 32.62 | 6 |
| | ATOM | 891 | CB | MET B 379 | -25.797 | 85.335 | 25.793 | 1.00 | 31.45 | 6 |
| 40 | ATOM | 892 | CG | MET B 379 | -27.332 | 85.262 | 25.883 | 1.00 | 38.75 | 6 |
| | ATOM | 893 | SD | MET B 379 | -28.020 | 86.915 | 25.550 | 1.00 | 41.27 | 16 |
| | ATOM | 894 | CE | MET B 379 | -29.814 | 86.586 | 25.513 | 1.00 | 35.68 | 6 |
| | ATOM | 895 | C | MET B 379 | -23.796 | 86.129 | 24.538 | 1.00 | 33.72 | 6 |
| | ATOM | 896 | O | MET B 379 | -23.246 | 86.190 | 25.633 | 1.00 | 36.29 | 8 |
| 45 | ATOM | 897 | N | SER B 380 | -23.152 | 86.335 | 23.399 | 1.00 | 34.49 | 7 |
| | ATOM | 898 | CA | SER B 380 | -21.738 | 86.659 | 23.391 | 1.00 | 33.97 | 6 |
| | ATOM | 899 | CB | SER B 380 | -21.132 | 86.360 | 22.010 | 1.00 | 31.24 | 6 |
| | ATOM | 900 | OG | SER B 380 | -21.224 | 84.978 | 21.696 | 1.00 | 39.42 | 8 |
| | ATOM | 901 | C | SER B 380 | -21.635 | 88.145 | 23.705 | 1.00 | 39.69 | 6 |
| 50 | ATOM | 902 | O | SER B 380 | -22.084 | 88.989 | 22.933 | 1.00 | 44.64 | 8 |
| | ATOM | 903 | N | SER B 381 | -21.053 | 88.451 | 24.857 | 1.00 | 41.04 | 7 |
| | ATOM | 904 | CA | SER B 381 | -20.907 | 89.826 | 25.308 | 1.00 | 44.91 | 6 |
| | ATOM | 905 | CB | SER B 381 | -20.610 | 89.832 | 26.797 | 1.00 | 44.50 | 6 |
| | ATOM | 906 | OG | SER B 381 | -19.351 | 89.229 | 27.037 | 1.00 | 45.42 | 8 |
| 55 | ATOM | 907 | C | SER B 381 | -19.815 | 90.614 | 24.602 | 1.00 | 44.59 | 6 |
| | ATOM | 908 | O | SER B 381 | -19.725 | 91.825 | 24.751 | 1.00 | 49.32 | 8 |
| | ATOM | 909 | N | ASP B 382 | -18.977 | 89.922 | 23.848 | 1.00 | 43.75 | 7 |
| | ATOM | 910 | CA | ASP B 382 | -17.886 | 90.556 | 23.144 | 1.00 | 43.93 | 6 |

| | | | | | | | | | | | | |
|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 911 | CB | ASP | B | 382 | -16.727 | 89.562 | 23.028 | 1.00 | 48.39 | 6 |
| | ATOM | 912 | CG | ASP | B | 382 | -17.142 | 88.232 | 22.471 | 1.00 | 53.23 | 6 |
| | ATOM | 913 | OD1 | ASP | B | 382 | -18.102 | 87.621 | 23.002 | 1.00 | 56.97 | 8 |
| | ATOM | 914 | OD2 | ASP | B | 382 | -16.513 | 87.753 | 21.480 | 1.00 | 58.91 | 8 |
| | ATOM | 915 | C | ASP | B | 382 | -18.191 | 91.172 | 21.772 | 1.00 | 41.09 | 6 |
| 10 | ATOM | 916 | O | ASP | B | 382 | -17.366 | 91.899 | 21.229 | 1.00 | 40.93 | 8 |
| | ATOM | 917 | N | ARG | B | 383 | -19.369 | 90.908 | 21.224 | 1.00 | 42.63 | 7 |
| | ATOM | 918 | CA | ARG | B | 383 | -19.698 | 91.445 | 19.934 | 1.00 | 43.32 | 6 |
| | ATOM | 919 | CB | ARG | B | 383 | -21.131 | 91.101 | 19.557 | 1.00 | 42.31 | 6 |
| | ATOM | 920 | CG | ARG | B | 383 | -21.619 | 89.672 | 19.811 | 1.00 | 40.83 | 6 |
| 15 | ATOM | 921 | CD | ARG | B | 383 | -21.144 | 88.627 | 18.804 | 1.00 | 38.09 | 6 |
| | ATOM | 922 | NE | ARG | B | 383 | -21.922 | 87.415 | 18.943 | 1.00 | 37.33 | 7 |
| | ATOM | 923 | CZ | ARG | B | 383 | -21.584 | 86.250 | 18.411 | 1.00 | 38.35 | 6 |
| | ATOM | 924 | NH1 | ARG | B | 383 | -20.465 | 86.143 | 17.700 | 1.00 | 33.70 | 7 |
| | ATOM | 925 | NH2 | ARG | B | 383 | -22.369 | 85.196 | 18.604 | 1.00 | 35.46 | 7 |
| 20 | ATOM | 926 | C | ARG | B | 383 | -19.591 | 92.958 | 20.007 | 1.00 | 44.96 | 6 |
| | ATOM | 927 | O | ARG | B | 383 | -20.050 | 93.577 | 20.980 | 1.00 | 45.60 | 8 |
| | ATOM | 928 | N | PRO | B | 384 | -18.975 | 93.579 | 19.005 | 1.00 | 45.33 | 7 |
| | ATOM | 929 | CD | PRO | B | 384 | -18.395 | 92.881 | 17.854 | 1.00 | 46.85 | 6 |
| | ATOM | 930 | CA | PRO | B | 384 | -18.808 | 95.035 | 18.947 | 1.00 | 47.37 | 6 |
| 25 | ATOM | 931 | CB | PRO | B | 384 | -17.868 | 95.255 | 17.764 | 1.00 | 46.90 | 6 |
| | ATOM | 932 | CG | PRO | B | 384 | -17.575 | 93.934 | 17.187 | 1.00 | 46.41 | 6 |
| | ATOM | 933 | C | PRO | B | 384 | -20.125 | 95.778 | 18.762 | 1.00 | 48.29 | 6 |
| | ATOM | 934 | O | PRO | B | 384 | -21.048 | 95.277 | 18.120 | 1.00 | 48.34 | 8 |
| | ATOM | 935 | N | GLY | B | 385 | -20.185 | 96.994 | 19.314 | 1.00 | 49.88 | 7 |
| 30 | ATOM | 936 | CA | GLY | B | 385 | -21.371 | 97.838 | 19.192 | 1.00 | 50.35 | 6 |
| | ATOM | 937 | C | GLY | B | 385 | -22.410 | 97.615 | 20.265 | 1.00 | 50.70 | 6 |
| | ATOM | 938 | O | GLY | B | 385 | -23.382 | 98.363 | 20.374 | 1.00 | 53.48 | 8 |
| | ATOM | 939 | N | LEU | B | 386 | -22.205 | 96.557 | 21.044 | 1.00 | 49.04 | 7 |
| | ATOM | 940 | CA | LEU | B | 386 | -23.136 | 96.211 | 22.101 | 1.00 | 50.53 | 6 |
| 35 | ATOM | 941 | CB | LEU | B | 386 | -22.640 | 94.972 | 22.853 | 1.00 | 45.17 | 6 |
| | ATOM | 942 | CG | LEU | B | 386 | -22.744 | 93.653 | 22.121 | 1.00 | 48.26 | 6 |
| | ATOM | 943 | CD1 | LEU | B | 386 | -22.122 | 92.525 | 22.938 | 1.00 | 41.68 | 6 |
| | ATOM | 944 | CD2 | LEU | B | 386 | -24.215 | 93.376 | 21.852 | 1.00 | 38.40 | 6 |
| | ATOM | 945 | C | LEU | B | 386 | -23.322 | 97.357 | 23.058 | 1.00 | 52.13 | 6 |
| 40 | ATOM | 946 | O | LEU | B | 386 | -22.438 | 98.182 | 23.234 | 1.00 | 53.67 | 8 |
| | ATOM | 947 | N | ALA | B | 387 | -24.499 | 97.398 | 23.666 | 1.00 | 53.42 | 7 |
| | ATOM | 948 | CA | ALA | B | 387 | -24.830 | 98.441 | 24.624 | 1.00 | 56.01 | 6 |
| | ATOM | 949 | CB | ALA | B | 387 | -26.223 | 98.993 | 24.339 | 1.00 | 56.47 | 6 |
| | ATOM | 950 | C | ALA | B | 387 | -24.775 | 97.853 | 26.024 | 1.00 | 55.52 | 6 |
| 45 | ATOM | 951 | O | ALA | B | 387 | -23.798 | 98.027 | 26.753 | 1.00 | 53.75 | 8 |
| | ATOM | 952 | N | CYS | B | 388 | -25.843 | 97.145 | 26.371 | 1.00 | 56.03 | 7 |
| | ATOM | 953 | CA | CYS | B | 388 | -26.000 | 96.525 | 27.673 | 1.00 | 59.57 | 6 |
| | ATOM | 954 | CB | CYS | B | 388 | -27.469 | 96.134 | 27.839 | 1.00 | 59.23 | 6 |
| | ATOM | 955 | SG | CYS | B | 388 | -28.620 | 97.392 | 27.264 | 1.00 | 58.64 | 16 |
| 50 | ATOM | 956 | C | CYS | B | 388 | -25.105 | 95.283 | 27.798 | 1.00 | 62.18 | 6 |
| | ATOM | 957 | O | CYS | B | 388 | -25.590 | 94.164 | 27.868 | 1.00 | 67.88 | 8 |
| | ATOM | 958 | N | VAL | B | 389 | -23.789 | 95.510 | 27.824 | 1.00 | 60.78 | 7 |
| | ATOM | 959 | CA | VAL | B | 389 | -22.797 | 94.434 | 27.959 | 1.00 | 57.70 | 6 |
| | ATOM | 960 | CB | VAL | B | 389 | -21.355 | 94.976 | 27.998 | 1.00 | 57.09 | 6 |
| 55 | ATOM | 961 | CG1 | VAL | B | 389 | -20.361 | 93.832 | 28.085 | 1.00 | 59.03 | 6 |
| | ATOM | 962 | CG2 | VAL | B | 389 | -21.065 | 95.845 | 26.791 | 1.00 | 53.98 | 6 |
| | ATOM | 963 | C | VAL | B | 389 | -23.078 | 93.642 | 29.230 | 1.00 | 57.77 | 6 |
| | ATOM | 964 | O | VAL | B | 389 | -23.727 | 92.602 | 29.203 | 1.00 | 60.94 | 8 |

| | | | | | | | | | | |
|----|------|------|-----|-----------|---------|--------|--------|------|-------|---|
| 5 | ATOM | 965 | N | ALA B 390 | -22.561 | 94.159 | 30.332 | 1.00 | 52.68 | 7 |
| | ATOM | 966 | CA | ALA B 390 | -22.684 | 93.570 | 31.659 | 1.00 | 48.41 | 6 |
| | ATOM | 967 | CB | ALA B 390 | -22.650 | 94.681 | 32.716 | 1.00 | 45.19 | 6 |
| | ATOM | 968 | C | ALA B 390 | -23.905 | 92.697 | 31.877 | 1.00 | 47.63 | 6 |
| | ATOM | 969 | O | ALA B 390 | -23.784 | 91.576 | 32.369 | 1.00 | 51.95 | 8 |
| 10 | ATOM | 970 | N | ARG B 391 | -25.075 | 93.216 | 31.498 | 1.00 | 47.11 | 7 |
| | ATOM | 971 | CA | ARG B 391 | -26.330 | 92.481 | 31.656 | 1.00 | 51.64 | 6 |
| | ATOM | 972 | CB | ARG B 391 | -27.502 | 93.318 | 31.122 | 1.00 | 54.22 | 6 |
| | ATOM | 973 | CG | ARG B 391 | -28.887 | 92.713 | 31.430 | 1.00 | 64.20 | 6 |
| | ATOM | 974 | CD | ARG B 391 | -30.059 | 93.582 | 30.929 | 1.00 | 73.80 | 6 |
| 15 | ATOM | 975 | NE | ARG B 391 | -31.361 | 93.097 | 31.378 | 1.00 | 79.76 | 7 |
| | ATOM | 976 | CZ | ARG B 391 | -31.736 | 93.015 | 32.656 | 1.00 | 84.27 | 6 |
| | ATOM | 977 | NH1 | ARG B 391 | -30.887 | 93.372 | 33.625 | 1.00 | 85.28 | 7 |
| | ATOM | 978 | NH2 | ARG B 391 | -32.957 | 92.566 | 32.955 | 1.00 | 86.84 | 7 |
| | ATOM | 979 | C | ARG B 391 | -26.277 | 91.133 | 30.940 | 1.00 | 48.18 | 6 |
| 20 | ATOM | 980 | O | ARG B 391 | -26.724 | 90.119 | 31.465 | 1.00 | 49.57 | 8 |
| | ATOM | 981 | N | ILE B 392 | -25.743 | 91.167 | 29.718 | 1.00 | 45.01 | 7 |
| | ATOM | 982 | CA | ILE B 392 | -25.592 | 89.999 | 28.867 | 1.00 | 48.77 | 6 |
| | ATOM | 983 | CB | ILE B 392 | -25.112 | 90.424 | 27.469 | 1.00 | 46.45 | 6 |
| | ATOM | 984 | CG2 | ILE B 392 | -24.805 | 89.221 | 26.614 | 1.00 | 42.35 | 6 |
| 25 | ATOM | 985 | CG1 | ILE B 392 | -26.178 | 91.283 | 26.768 | 1.00 | 49.69 | 6 |
| | ATOM | 986 | CD1 | ILE B 392 | -25.762 | 91.768 | 25.386 | 1.00 | 51.09 | 6 |
| | ATOM | 987 | C | ILE B 392 | -24.671 | 88.935 | 29.462 | 1.00 | 50.90 | 6 |
| | ATOM | 988 | O | ILE B 392 | -25.086 | 87.780 | 29.605 | 1.00 | 52.21 | 8 |
| | ATOM | 989 | N | GLU B 393 | -23.431 | 89.298 | 29.790 | 1.00 | 50.43 | 7 |
| 30 | ATOM | 990 | CA | GLU B 393 | -22.504 | 88.328 | 30.378 | 1.00 | 50.30 | 6 |
| | ATOM | 991 | CB | GLU B 393 | -21.314 | 89.022 | 31.044 | 1.00 | 53.97 | 6 |
| | ATOM | 992 | CG | GLU B 393 | -20.063 | 89.005 | 30.209 | 1.00 | 62.18 | 6 |
| | ATOM | 993 | CD | GLU B 393 | -18.877 | 89.415 | 30.976 | 1.00 | 67.69 | 6 |
| | ATOM | 994 | OE1 | GLU B 393 | -17.709 | 89.264 | 30.656 | 1.00 | 66.42 | 8 |
| 35 | ATOM | 995 | OE2 | GLU B 393 | -18.897 | 89.976 | 32.052 | 1.00 | 70.64 | 8 |
| | ATOM | 996 | C | GLU B 393 | -23.251 | 87.477 | 31.416 | 1.00 | 49.31 | 6 |
| | ATOM | 997 | O | GLU B 393 | -23.226 | 86.260 | 31.303 | 1.00 | 49.53 | 8 |
| | ATOM | 998 | N | LYS B 394 | -23.898 | 88.153 | 32.409 | 1.00 | 46.07 | 7 |
| | ATOM | 999 | CA | LYS B 394 | -24.721 | 87.579 | 33.506 | 1.00 | 45.76 | 6 |
| 40 | ATOM | 1000 | CB | LYS B 394 | -25.594 | 88.693 | 34.161 | 1.00 | 43.85 | 6 |
| | ATOM | 1001 | C | LYS B 394 | -25.626 | 86.548 | 32.851 | 1.00 | 46.69 | 6 |
| | ATOM | 1002 | O | LYS B 394 | -25.772 | 85.430 | 33.329 | 1.00 | 49.13 | 8 |
| | ATOM | 1003 | N | TYR B 395 | -26.203 | 86.948 | 31.719 | 1.00 | 46.57 | 7 |
| | ATOM | 1004 | CA | TYR B 395 | -27.076 | 86.078 | 30.938 | 1.00 | 43.33 | 6 |
| 45 | ATOM | 1005 | CB | TYR B 395 | -27.621 | 86.821 | 29.716 | 1.00 | 48.44 | 6 |
| | ATOM | 1006 | CG | TYR B 395 | -28.827 | 87.688 | 29.980 | 1.00 | 53.83 | 6 |
| | ATOM | 1007 | CD1 | TYR B 395 | -29.204 | 88.680 | 29.080 | 1.00 | 56.43 | 6 |
| | ATOM | 1008 | CE1 | TYR B 395 | -30.331 | 89.469 | 29.309 | 1.00 | 59.73 | 6 |
| | ATOM | 1009 | CD2 | TYR B 395 | -29.596 | 87.509 | 31.113 | 1.00 | 56.47 | 6 |
| 50 | ATOM | 1010 | CE2 | TYR B 395 | -30.723 | 88.295 | 31.346 | 1.00 | 62.60 | 6 |
| | ATOM | 1011 | CZ | TYR B 395 | -31.090 | 89.281 | 30.446 | 1.00 | 63.18 | 6 |
| | ATOM | 1012 | OH | TYR B 395 | -32.189 | 90.068 | 30.671 | 1.00 | 64.46 | 8 |
| | ATOM | 1013 | C | TYR B 395 | -26.276 | 84.867 | 30.485 | 1.00 | 37.30 | 6 |
| | ATOM | 1014 | O | TYR B 395 | -26.611 | 83.737 | 30.825 | 1.00 | 34.10 | 8 |
| 55 | ATOM | 1015 | N | GLN B 396 | -25.213 | 85.108 | 29.718 | 1.00 | 31.92 | 7 |
| | ATOM | 1016 | CA | GLN B 396 | -24.380 | 84.018 | 29.244 | 1.00 | 34.81 | 6 |
| | ATOM | 1017 | CB | GLN B 396 | -23.176 | 84.550 | 28.464 | 1.00 | 32.64 | 6 |
| | ATOM | 1018 | CG | GLN B 396 | -22.184 | 83.470 | 28.103 | 1.00 | 29.57 | 6 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 1019 | CD | GLN | B | 396 | -21.214 | 83.871 | 27.016 | 1.00 | 29.46 | 6 |
| | ATOM | 1020 | OE1 | GLN | B | 396 | -20.547 | 84.930 | 27.109 | 1.00 | 34.65 | 8 |
| | ATOM | 1021 | NE2 | GLN | B | 396 | -21.112 | 83.032 | 25.992 | 1.00 | 27.21 | 7 |
| | ATOM | 1022 | C | GLN | B | 396 | -23.908 | 83.207 | 30.434 | 1.00 | 37.13 | 6 |
| | ATOM | 1023 | O | GLN | B | 396 | -23.876 | 81.986 | 30.384 | 1.00 | 37.36 | 8 |
| 10 | ATOM | 1024 | N | ASP | B | 397 | -23.544 | 83.903 | 31.508 | 1.00 | 38.61 | 7 |
| | ATOM | 1025 | CA | ASP | B | 397 | -23.069 | 83.250 | 32.717 | 1.00 | 40.37 | 6 |
| | ATOM | 1026 | CB | ASP | B | 397 | -22.617 | 84.297 | 33.754 | 1.00 | 40.51 | 6 |
| | ATOM | 1027 | CG | ASP | B | 397 | -21.360 | 85.025 | 33.352 | 1.00 | 43.77 | 6 |
| | ATOM | 1028 | OD1 | ASP | B | 397 | -20.337 | 84.366 | 33.054 | 1.00 | 46.50 | 8 |
| 15 | ATOM | 1029 | OD2 | ASP | B | 397 | -21.343 | 86.287 | 33.350 | 1.00 | 51.34 | 8 |
| | ATOM | 1030 | C | ASP | B | 397 | -24.223 | 82.422 | 33.267 | 1.00 | 38.62 | 6 |
| | ATOM | 1031 | O | ASP | B | 397 | -24.023 | 81.327 | 33.778 | 1.00 | 39.20 | 8 |
| | ATOM | 1032 | N | SER | B | 398 | -25.432 | 82.962 | 33.138 | 1.00 | 37.84 | 7 |
| | ATOM | 1033 | CA | SER | B | 398 | -26.633 | 82.293 | 33.622 | 1.00 | 37.80 | 6 |
| 20 | ATOM | 1034 | CB | SER | B | 398 | -27.830 | 83.246 | 33.501 | 1.00 | 34.28 | 6 |
| | ATOM | 1035 | OG | SER | B | 398 | -28.995 | 82.715 | 34.114 | 1.00 | 46.60 | 8 |
| | ATOM | 1036 | C | SER | B | 398 | -26.911 | 80.997 | 32.867 | 1.00 | 38.41 | 6 |
| | ATOM | 1037 | O | SER | B | 398 | -27.454 | 80.047 | 33.433 | 1.00 | 39.98 | 8 |
| | ATOM | 1038 | N | PHE | B | 399 | -26.546 | 80.963 | 31.587 | 1.00 | 34.82 | 7 |
| 25 | ATOM | 1039 | CA | PHE | B | 399 | -26.772 | 79.768 | 30.781 | 1.00 | 35.96 | 6 |
| | ATOM | 1040 | CB | PHE | B | 399 | -26.892 | 80.100 | 29.293 | 1.00 | 35.75 | 6 |
| | ATOM | 1041 | CG | PHE | B | 399 | -28.211 | 80.717 | 28.906 | 1.00 | 39.30 | 6 |
| | ATOM | 1042 | CD1 | PHE | B | 399 | -28.466 | 82.056 | 29.109 | 1.00 | 39.86 | 6 |
| | ATOM | 1043 | CD2 | PHE | B | 399 | -29.194 | 79.938 | 28.355 | 1.00 | 36.81 | 6 |
| 30 | ATOM | 1044 | CE1 | PHE | B | 399 | -29.700 | 82.602 | 28.739 | 1.00 | 41.25 | 6 |
| | ATOM | 1045 | CE2 | PHE | B | 399 | -30.424 | 80.483 | 27.987 | 1.00 | 43.61 | 6 |
| | ATOM | 1046 | CZ | PHE | B | 399 | -30.677 | 81.813 | 28.181 | 1.00 | 40.34 | 6 |
| | ATOM | 1047 | C | PHE | B | 399 | -25.658 | 78.754 | 30.976 | 1.00 | 33.48 | 6 |
| | ATOM | 1048 | O | PHE | B | 399 | -25.927 | 77.589 | 31.256 | 1.00 | 26.86 | 8 |
| 35 | ATOM | 1049 | N | LEU | B | 400 | -24.408 | 79.187 | 30.796 | 1.00 | 31.47 | 7 |
| | ATOM | 1050 | CA | LEU | B | 400 | -23.275 | 78.291 | 30.945 | 1.00 | 37.41 | 6 |
| | ATOM | 1051 | CB | LEU | B | 400 | -21.976 | 79.091 | 31.030 | 1.00 | 34.24 | 6 |
| | ATOM | 1052 | CG | LEU | B | 400 | -21.470 | 79.642 | 29.726 | 1.00 | 35.10 | 6 |
| | ATOM | 1053 | CD1 | LEU | B | 400 | -20.121 | 80.304 | 29.917 | 1.00 | 26.60 | 6 |
| 40 | ATOM | 1054 | CD2 | LEU | B | 400 | -21.326 | 78.488 | 28.759 | 1.00 | 29.44 | 6 |
| | ATOM | 1055 | C | LEU | B | 400 | -23.430 | 77.376 | 32.145 | 1.00 | 38.84 | 6 |
| | ATOM | 1056 | O | LEU | B | 400 | -23.366 | 76.157 | 32.007 | 1.00 | 40.38 | 8 |
| | ATOM | 1057 | N | LEU | B | 401 | -23.639 | 77.968 | 33.321 | 1.00 | 42.79 | 7 |
| | ATOM | 1058 | CA | LEU | B | 401 | -23.801 | 77.181 | 34.537 | 1.00 | 43.48 | 6 |
| 45 | ATOM | 1059 | CB | LEU | B | 401 | -24.226 | 78.067 | 35.712 | 1.00 | 44.73 | 6 |
| | ATOM | 1060 | CG | LEU | B | 401 | -24.378 | 77.303 | 37.012 | 1.00 | 51.39 | 6 |
| | ATOM | 1061 | CD1 | LEU | B | 401 | -22.990 | 76.844 | 37.484 | 1.00 | 50.11 | 6 |
| | ATOM | 1062 | CD2 | LEU | B | 401 | -25.027 | 78.163 | 38.083 | 1.00 | 49.30 | 6 |
| | ATOM | 1063 | C | LEU | B | 401 | -24.854 | 76.095 | 34.311 | 1.00 | 41.62 | 6 |
| 50 | ATOM | 1064 | O | LEU | B | 401 | -24.576 | 74.900 | 34.427 | 1.00 | 45.14 | 8 |
| | ATOM | 1065 | N | ALA | B | 402 | -26.068 | 76.532 | 33.997 | 1.00 | 37.92 | 7 |
| | ATOM | 1066 | CA | ALA | B | 402 | -27.177 | 75.631 | 33.752 | 1.00 | 29.90 | 6 |
| | ATOM | 1067 | CB | ALA | B | 402 | -28.361 | 76.433 | 33.200 | 1.00 | 30.70 | 6 |
| | ATOM | 1068 | C | ALA | B | 402 | -26.779 | 74.521 | 32.773 | 1.00 | 28.88 | 6 |
| 55 | ATOM | 1069 | O | ALA | B | 402 | -27.078 | 73.347 | 32.996 | 1.00 | 32.14 | 8 |
| | ATOM | 1070 | N | PHE | B | 403 | -26.091 | 74.908 | 31.698 | 1.00 | 31.07 | 7 |
| | ATOM | 1071 | CA | PHE | B | 403 | -25.655 | 73.970 | 30.673 | 1.00 | 29.90 | 6 |
| | ATOM | 1072 | CB | PHE | B | 403 | -24.847 | 74.715 | 29.607 | 1.00 | 27.03 | 6 |

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|----|------|------|-----|-------|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 1073 | CG | PHE B | 403 | -24.557 | 73.904 | 27.272 | 1.00 | 25.55 | 6 |
| | ATOM | 1074 | CD1 | PHE B | 403 | -23.916 | 74.494 | 27.272 | 1.00 | 25.55 | 6 |
| | ATOM | 1075 | CD2 | PHE B | 403 | -24.939 | 72.583 | 28.271 | 1.00 | 19.75 | 6 |
| | ATOM | 1076 | CE1 | PHE B | 403 | -23.670 | 73.765 | 26.104 | 1.00 | 27.90 | 6 |
| | ATOM | 1077 | CE2 | PHE B | 403 | -24.693 | 71.848 | 27.102 | 1.00 | 22.56 | 6 |
| 10 | ATOM | 1078 | CZ | PHE B | 403 | -24.057 | 72.439 | 26.020 | 1.00 | 22.24 | 6 |
| | ATOM | 1079 | C | PHE B | 403 | -24.810 | 72.902 | 31.329 | 1.00 | 28.82 | 6 |
| | ATOM | 1080 | O | PHE B | 403 | -25.092 | 71.726 | 31.205 | 1.00 | 26.00 | 8 |
| | ATOM | 1081 | N | GLU B | 404 | -23.776 | 73.335 | 32.037 | 1.00 | 30.25 | 7 |
| | ATOM | 1082 | CA | GLU B | 404 | -22.865 | 72.419 | 32.712 | 1.00 | 34.03 | 6 |
| 15 | ATOM | 1083 | CB | GLU B | 404 | -21.835 | 73.215 | 33.527 | 1.00 | 39.45 | 6 |
| | ATOM | 1084 | CG | GLU B | 404 | -20.654 | 72.384 | 34.068 | 1.00 | 47.68 | 6 |
| | ATOM | 1085 | CD | GLU B | 404 | -19.750 | 73.129 | 34.996 | 1.00 | 54.02 | 6 |
| | ATOM | 1086 | OE1 | GLU B | 404 | -19.372 | 74.290 | 34.701 | 1.00 | 57.27 | 8 |
| | ATOM | 1087 | OE2 | GLU B | 404 | -19.369 | 72.555 | 36.048 | 1.00 | 63.85 | 8 |
| 20 | ATOM | 1088 | C | GLU B | 404 | -23.645 | 71.509 | 33.642 | 1.00 | 36.01 | 6 |
| | ATOM | 1089 | O | GLU B | 404 | -23.470 | 70.292 | 33.640 | 1.00 | 38.64 | 8 |
| | ATOM | 1090 | N | HIS B | 405 | -24.492 | 72.131 | 34.458 | 1.00 | 29.56 | 7 |
| | ATOM | 1091 | CA | HIS B | 405 | -25.306 | 71.387 | 35.405 | 1.00 | 31.69 | 6 |
| | ATOM | 1092 | CB | HIS B | 405 | -26.245 | 72.324 | 36.173 | 1.00 | 33.75 | 6 |
| 25 | ATOM | 1093 | CG | HIS B | 405 | -25.536 | 73.185 | 37.163 | 1.00 | 34.75 | 6 |
| | ATOM | 1094 | CD2 | HIS B | 405 | -24.234 | 73.286 | 37.524 | 1.00 | 34.58 | 6 |
| | ATOM | 1095 | ND1 | HIS B | 405 | -26.223 | 74.101 | 37.969 | 1.00 | 32.43 | 7 |
| | ATOM | 1096 | CE1 | HIS B | 405 | -25.334 | 74.703 | 38.769 | 1.00 | 36.15 | 6 |
| | ATOM | 1097 | NE2 | HIS B | 405 | -24.139 | 74.222 | 38.511 | 1.00 | 39.84 | 7 |
| 30 | ATOM | 1098 | C | HIS B | 405 | -26.106 | 70.342 | 34.648 | 1.00 | 34.21 | 6 |
| | ATOM | 1099 | O | HIS B | 405 | -26.087 | 69.160 | 35.006 | 1.00 | 37.06 | 8 |
| | ATOM | 1100 | N | TYR B | 406 | -26.806 | 70.776 | 33.598 | 1.00 | 30.83 | 7 |
| | ATOM | 1101 | CA | TYR B | 406 | -27.592 | 69.853 | 32.796 | 1.00 | 28.85 | 6 |
| | ATOM | 1102 | CB | TYR B | 406 | -28.192 | 70.537 | 31.579 | 1.00 | 31.48 | 6 |
| 35 | ATOM | 1103 | CG | TYR B | 406 | -28.991 | 69.576 | 30.730 | 1.00 | 23.49 | 6 |
| | ATOM | 1104 | CD1 | TYR B | 406 | -30.179 | 69.047 | 31.196 | 1.00 | 19.42 | 6 |
| | ATOM | 1105 | CE1 | TYR B | 406 | -30.893 | 68.128 | 30.441 | 1.00 | 23.80 | 6 |
| | ATOM | 1106 | CD2 | TYR B | 406 | -28.525 | 69.152 | 29.496 | 1.00 | 21.81 | 6 |
| | ATOM | 1107 | CE2 | TYR B | 406 | -29.241 | 68.228 | 28.740 | 1.00 | 24.64 | 6 |
| 40 | ATOM | 1108 | CZ | TYR B | 406 | -30.420 | 67.713 | 29.217 | 1.00 | 21.56 | 6 |
| | ATOM | 1109 | OH | TYR B | 406 | -31.120 | 66.802 | 28.480 | 1.00 | 24.96 | 8 |
| | ATOM | 1110 | C | TYR B | 406 | -26.697 | 68.725 | 32.304 | 1.00 | 24.24 | 6 |
| | ATOM | 1111 | O | TYR B | 406 | -27.155 | 67.609 | 32.110 | 1.00 | 27.08 | 8 |
| | ATOM | 1112 | N | ILE B | 407 | -25.422 | 69.056 | 32.084 | 1.00 | 25.76 | 7 |
| 45 | ATOM | 1113 | CA | ILE B | 407 | -24.428 | 68.092 | 31.628 | 1.00 | 33.75 | 6 |
| | ATOM | 1114 | CB | ILE B | 407 | -23.090 | 68.778 | 31.274 | 1.00 | 34.23 | 6 |
| | ATOM | 1115 | CG2 | ILE B | 407 | -21.959 | 67.774 | 31.230 | 1.00 | 32.46 | 6 |
| | ATOM | 1116 | CG1 | ILE B | 407 | -23.214 | 69.514 | 29.936 | 1.00 | 43.30 | 6 |
| | ATOM | 1117 | CD1 | ILE B | 407 | -23.655 | 68.612 | 28.804 | 1.00 | 40.40 | 6 |
| 50 | ATOM | 1118 | C | ILE B | 407 | -24.191 | 67.004 | 32.658 | 1.00 | 39.03 | 6 |
| | ATOM | 1119 | O | ILE B | 407 | -24.178 | 65.806 | 32.343 | 1.00 | 35.18 | 8 |
| | ATOM | 1120 | N | ASN B | 408 | -23.990 | 67.425 | 33.894 | 1.00 | 37.25 | 7 |
| | ATOM | 1121 | CA | ASN B | 408 | -23.739 | 66.475 | 34.943 | 1.00 | 37.01 | 6 |
| | ATOM | 1122 | CB | ASN B | 408 | -23.524 | 67.221 | 36.256 | 1.00 | 32.27 | 6 |
| 55 | ATOM | 1123 | CG | ASN B | 408 | -22.296 | 68.137 | 36.202 | 1.00 | 33.56 | 6 |
| | ATOM | 1124 | OD1 | ASN B | 408 | -21.194 | 67.696 | 35.823 | 1.00 | 31.99 | 8 |
| | ATOM | 1125 | ND2 | ASN B | 408 | -22.478 | 69.397 | 36.604 | 1.00 | 31.23 | 7 |
| | ATOM | 1126 | C | ASN B | 408 | -24.876 | 65.453 | 35.036 | 1.00 | 38.14 | 6 |

| | | | | | | | | | | |
|----|------|------|-----|-----------|---------|--------|--------|------|-------|---|
| 5 | ATOM | 1127 | O | ASN B 408 | -24.624 | 64.253 | 35.105 | 1.00 | 42.16 | 8 |
| | ATOM | 1128 | N | TYR B 409 | -26.122 | 65.924 | 35.003 | 1.00 | 35.62 | 7 |
| | ATOM | 1129 | CA | TYR B 409 | -27.273 | 65.024 | 35.073 | 1.00 | 35.91 | 6 |
| | ATOM | 1130 | CB | TYR B 409 | -28.597 | 65.787 | 34.931 | 1.00 | 34.41 | 6 |
| | ATOM | 1131 | CG | TYR B 409 | -29.788 | 64.868 | 34.685 | 1.00 | 38.73 | 6 |
| 10 | ATOM | 1132 | CD1 | TYR B 409 | -30.064 | 63.819 | 35.549 | 1.00 | 41.34 | 6 |
| | ATOM | 1133 | CE1 | TYR B 409 | -31.130 | 62.962 | 35.309 | 1.00 | 47.16 | 6 |
| | ATOM | 1134 | CD2 | TYR B 409 | -30.613 | 65.037 | 33.579 | 1.00 | 46.20 | 6 |
| | ATOM | 1135 | CE2 | TYR B 409 | -31.684 | 64.176 | 33.341 | 1.00 | 50.74 | 6 |
| | ATOM | 1136 | CZ | TYR B 409 | -31.942 | 63.143 | 34.206 | 1.00 | 50.88 | 6 |
| 15 | ATOM | 1137 | OH | TYR B 409 | -33.002 | 62.312 | 33.978 | 1.00 | 53.14 | 8 |
| | ATOM | 1138 | C | TYR B 409 | -27.215 | 64.020 | 33.951 | 1.00 | 38.16 | 6 |
| | ATOM | 1139 | O | TYR B 409 | -27.558 | 62.857 | 34.111 | 1.00 | 41.83 | 8 |
| | ATOM | 1140 | N | ARG B 410 | -26.824 | 64.528 | 32.796 | 1.00 | 42.25 | 7 |
| | ATOM | 1141 | CA | ARG B 410 | -26.734 | 63.739 | 31.594 | 1.00 | 42.83 | 6 |
| 20 | ATOM | 1142 | CB | ARG B 410 | -26.350 | 64.646 | 30.441 | 1.00 | 36.83 | 6 |
| | ATOM | 1143 | CG | ARG B 410 | -27.440 | 65.585 | 29.945 | 1.00 | 34.32 | 6 |
| | ATOM | 1144 | CD | ARG B 410 | -28.284 | 64.863 | 28.917 | 1.00 | 36.62 | 6 |
| | ATOM | 1145 | NE | ARG B 410 | -27.455 | 64.378 | 27.829 | 1.00 | 38.64 | 7 |
| | ATOM | 1146 | CZ | ARG B 410 | -27.926 | 63.656 | 26.824 | 1.00 | 35.73 | 6 |
| 25 | ATOM | 1147 | NH1 | ARG B 410 | -29.234 | 63.379 | 26.782 | 1.00 | 33.17 | 7 |
| | ATOM | 1148 | NH2 | ARG B 410 | -27.095 | 63.227 | 25.868 | 1.00 | 32.70 | 7 |
| | ATOM | 1149 | C | ARG B 410 | -25.688 | 62.664 | 31.733 | 1.00 | 46.67 | 6 |
| | ATOM | 1150 | O | ARG B 410 | -25.859 | 61.547 | 31.257 | 1.00 | 41.78 | 8 |
| | ATOM | 1151 | N | LYS B 411 | -24.602 | 63.028 | 32.413 | 1.00 | 52.99 | 7 |
| 30 | ATOM | 1152 | CA | LYS B 411 | -23.471 | 62.145 | 32.609 | 1.00 | 58.32 | 6 |
| | ATOM | 1153 | CB | LYS B 411 | -23.684 | 61.249 | 33.833 | 1.00 | 64.99 | 6 |
| | ATOM | 1154 | CG | LYS B 411 | -24.998 | 60.544 | 33.968 | 1.00 | 70.48 | 6 |
| | ATOM | 1155 | CD | LYS B 411 | -25.070 | 59.887 | 35.349 | 1.00 | 77.18 | 6 |
| | ATOM | 1156 | CE | LYS B 411 | -26.272 | 58.944 | 35.474 | 1.00 | 84.30 | 6 |
| 35 | ATOM | 1157 | NZ | LYS B 411 | -26.286 | 58.242 | 36.809 | 1.00 | 86.48 | 7 |
| | ATOM | 1158 | C | LYS B 411 | -23.172 | 61.341 | 31.365 | 1.00 | 56.66 | 6 |
| | ATOM | 1159 | O | LYS B 411 | -23.574 | 60.199 | 31.210 | 1.00 | 55.47 | 8 |
| | ATOM | 1160 | N | HIS B 412 | -22.458 | 62.026 | 30.479 | 1.00 | 54.67 | 7 |
| | ATOM | 1161 | CA | HIS B 412 | -22.019 | 61.474 | 29.214 | 1.00 | 48.67 | 6 |
| 40 | ATOM | 1162 | CB | HIS B 412 | -21.500 | 62.599 | 28.310 | 1.00 | 43.14 | 6 |
| | ATOM | 1163 | CG | HIS B 412 | -22.559 | 63.501 | 27.784 | 1.00 | 41.36 | 6 |
| | ATOM | 1164 | CD2 | HIS B 412 | -23.159 | 64.603 | 28.299 | 1.00 | 35.44 | 6 |
| | ATOM | 1165 | ND1 | HIS B 412 | -23.163 | 63.290 | 26.539 | 1.00 | 38.19 | 7 |
| | ATOM | 1166 | CE1 | HIS B 412 | -24.076 | 64.238 | 26.353 | 1.00 | 34.75 | 6 |
| 45 | ATOM | 1167 | NE2 | HIS B 412 | -24.090 | 65.034 | 27.396 | 1.00 | 35.52 | 7 |
| | ATOM | 1168 | C | HIS B 412 | -20.894 | 60.596 | 29.644 | 1.00 | 46.35 | 6 |
| | ATOM | 1169 | O | HIS B 412 | -20.218 | 60.892 | 30.644 | 1.00 | 42.73 | 8 |
| | ATOM | 1170 | N | HIS B 413 | -20.708 | 59.469 | 28.973 | 1.00 | 48.92 | 7 |
| | ATOM | 1171 | CA | HIS B 413 | -19.593 | 58.614 | 29.371 | 1.00 | 53.15 | 6 |
| 50 | ATOM | 1172 | CB | HIS B 413 | -20.022 | 57.147 | 29.421 | 1.00 | 55.27 | 6 |
| | ATOM | 1173 | CG | HIS B 413 | -20.814 | 56.823 | 30.636 | 1.00 | 58.77 | 6 |
| | ATOM | 1174 | CD2 | HIS B 413 | -22.019 | 56.223 | 30.822 | 1.00 | 61.65 | 6 |
| | ATOM | 1175 | ND1 | HIS B 413 | -20.360 | 57.159 | 31.921 | 1.00 | 60.31 | 7 |
| | ATOM | 1176 | CE1 | HIS B 413 | -21.267 | 56.758 | 32.809 | 1.00 | 63.01 | 6 |
| 55 | ATOM | 1177 | NE2 | HIS B 413 | -22.270 | 56.193 | 32.171 | 1.00 | 62.93 | 7 |
| | ATOM | 1178 | C | HIS B 413 | -18.426 | 58.862 | 28.438 | 1.00 | 53.19 | 6 |
| | ATOM | 1179 | O | HIS B 413 | -17.975 | 57.996 | 27.699 | 1.00 | 54.93 | 8 |
| | ATOM | 1180 | N | VAL B 414 | -17.970 | 60.113 | 28.521 | 1.00 | 53.77 | 7 |

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|----|------|------|-----|-----------|---------|--------|--------|------|-------|---|
| 5 | ATOM | 1181 | CA | VAL B 414 | -16.845 | 60.674 | 27.788 | 1.00 | 51.06 | 6 |
| | ATOM | 1182 | CB | VAL B 414 | -17.317 | 61.498 | 26.586 | 1.00 | 51.49 | 6 |
| | ATOM | 1183 | CG1 | VAL B 414 | -16.133 | 62.122 | 25.891 | 1.00 | 45.22 | 6 |
| | ATOM | 1184 | CG2 | VAL B 414 | -18.095 | 60.631 | 25.617 | 1.00 | 52.67 | 6 |
| | ATOM | 1185 | C | VAL B 414 | -16.096 | 61.557 | 28.775 | 1.00 | 54.28 | 6 |
| 10 | ATOM | 1186 | O | VAL B 414 | -16.700 | 62.283 | 29.574 | 1.00 | 55.49 | 8 |
| | ATOM | 1187 | N | THR B 415 | -14.770 | 61.466 | 28.742 | 1.00 | 56.28 | 7 |
| | ATOM | 1188 | CA | THR B 415 | -13.919 | 62.234 | 29.669 | 1.00 | 57.83 | 6 |
| | ATOM | 1189 | CB | THR B 415 | -12.488 | 61.686 | 29.658 | 1.00 | 59.64 | 6 |
| | ATOM | 1190 | OG1 | THR B 415 | -11.618 | 62.572 | 30.373 | 1.00 | 66.69 | 8 |
| 15 | ATOM | 1191 | CG2 | THR B 415 | -11.988 | 61.483 | 28.227 | 1.00 | 59.42 | 6 |
| | ATOM | 1192 | C | THR B 415 | -13.840 | 63.726 | 29.352 | 1.00 | 56.98 | 6 |
| | ATOM | 1193 | O | THR B 415 | -13.987 | 64.135 | 28.216 | 1.00 | 55.70 | 8 |
| | ATOM | 1194 | N | HIS B 416 | -13.598 | 64.522 | 30.387 | 1.00 | 57.44 | 7 |
| | ATOM | 1195 | CA | HIS B 416 | -13.485 | 65.972 | 30.237 | 1.00 | 57.34 | 6 |
| 20 | ATOM | 1196 | CB | HIS B 416 | -12.114 | 66.326 | 29.653 | 1.00 | 61.35 | 6 |
| | ATOM | 1197 | CG | HIS B 416 | -10.968 | 65.931 | 30.513 | 1.00 | 69.78 | 6 |
| | ATOM | 1198 | CD2 | HIS B 416 | -9.930 | 65.082 | 30.307 | 1.00 | 71.42 | 6 |
| | ATOM | 1199 | ND1 | HIS B 416 | -10.756 | 66.480 | 31.787 | 1.00 | 72.49 | 7 |
| | ATOM | 1200 | CE1 | HIS B 416 | -9.631 | 65.973 | 32.281 | 1.00 | 75.50 | 6 |
| 25 | ATOM | 1201 | NE2 | HIS B 416 | -9.120 | 65.131 | 31.408 | 1.00 | 73.91 | 7 |
| | ATOM | 1202 | C | HIS B 416 | -14.560 | 66.515 | 29.320 | 1.00 | 53.79 | 6 |
| | ATOM | 1203 | O | HIS B 416 | -14.334 | 67.477 | 28.591 | 1.00 | 52.81 | 8 |
| | ATOM | 1204 | N | PHE B 417 | -15.746 | 65.921 | 29.372 | 1.00 | 48.05 | 7 |
| | ATOM | 1205 | CA | PHE B 417 | -16.841 | 66.329 | 28.505 | 1.00 | 47.99 | 6 |
| 30 | ATOM | 1206 | CB | PHE B 417 | -18.152 | 65.694 | 28.937 | 1.00 | 46.11 | 6 |
| | ATOM | 1207 | CG | PHE B 417 | -19.233 | 65.781 | 27.898 | 1.00 | 44.27 | 6 |
| | ATOM | 1208 | CD1 | PHE B 417 | -19.280 | 64.856 | 26.870 | 1.00 | 41.79 | 6 |
| | ATOM | 1209 | CD2 | PHE B 417 | -20.118 | 66.846 | 27.893 | 1.00 | 40.23 | 6 |
| | ATOM | 1210 | CE1 | PHE B 417 | -20.233 | 64.959 | 25.869 | 1.00 | 44.30 | 6 |
| 35 | ATOM | 1211 | CE2 | PHE B 417 | -21.072 | 66.955 | 26.893 | 1.00 | 36.80 | 6 |
| | ATOM | 1212 | CZ | PHE B 417 | -21.119 | 66.016 | 25.866 | 1.00 | 40.69 | 6 |
| | ATOM | 1213 | C | PHE B 417 | -17.020 | 67.833 | 28.423 | 1.00 | 46.69 | 6 |
| | ATOM | 1214 | O | PHE B 417 | -16.799 | 68.423 | 27.380 | 1.00 | 43.35 | 8 |
| | ATOM | 1215 | N | TRP B 418 | -17.448 | 68.452 | 29.516 | 1.00 | 45.14 | 7 |
| 40 | ATOM | 1216 | CA | TRP B 418 | -17.681 | 69.889 | 29.508 | 1.00 | 44.89 | 6 |
| | ATOM | 1217 | CB | TRP B 418 | -18.045 | 70.398 | 30.898 | 1.00 | 42.24 | 6 |
| | ATOM | 1218 | CG | TRP B 418 | -18.162 | 71.905 | 31.018 | 1.00 | 47.11 | 6 |
| | ATOM | 1219 | CD2 | TRP B 418 | -19.298 | 72.699 | 30.620 | 1.00 | 46.98 | 6 |
| | ATOM | 1220 | CE2 | TRP B 418 | -18.953 | 74.061 | 30.850 | 1.00 | 48.94 | 6 |
| 45 | ATOM | 1221 | CE3 | TRP B 418 | -20.560 | 72.401 | 30.086 | 1.00 | 45.23 | 6 |
| | ATOM | 1222 | CD1 | TRP B 418 | -17.223 | 72.778 | 31.462 | 1.00 | 46.24 | 6 |
| | ATOM | 1223 | NE1 | TRP B 418 | -17.690 | 74.071 | 31.368 | 1.00 | 50.63 | 7 |
| | ATOM | 1224 | CZ2 | TRP B 418 | -19.819 | 75.109 | 30.571 | 1.00 | 45.46 | 6 |
| | ATOM | 1225 | CZ3 | TRP B 418 | -21.422 | 73.447 | 29.809 | 1.00 | 44.50 | 6 |
| 50 | ATOM | 1226 | CH2 | TRP B 418 | -21.065 | 74.777 | 30.039 | 1.00 | 47.55 | 6 |
| | ATOM | 1227 | C | TRP B 418 | -16.502 | 70.662 | 28.956 | 1.00 | 43.88 | 6 |
| | ATOM | 1228 | O | TRP B 418 | -16.671 | 71.424 | 27.986 | 1.00 | 43.17 | 8 |
| | ATOM | 1229 | N | PRO B 419 | -15.292 | 70.490 | 29.519 | 1.00 | 43.55 | 7 |
| | ATOM | 1230 | CD | PRO B 419 | -14.967 | 69.551 | 30.599 | 1.00 | 41.52 | 6 |
| 55 | ATOM | 1231 | CA | PRO B 419 | -14.120 | 71.223 | 29.011 | 1.00 | 41.48 | 6 |
| | ATOM | 1232 | CB | PRO B 419 | -12.956 | 70.582 | 29.724 | 1.00 | 39.21 | 6 |
| | ATOM | 1233 | CG | PRO B 419 | -13.521 | 69.703 | 30.774 | 1.00 | 39.25 | 6 |
| | ATOM | 1234 | C | PRO B 419 | -14.035 | 71.067 | 27.479 | 1.00 | 36.28 | 6 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 1235 | O | PRO | B | 419 | -13.690 | 72.001 | 26.754 | 1.00 | 37.08 | 8 |
| | ATOM | 1236 | N | LYS | B | 420 | -14.330 | 69.871 | 26.976 | 1.00 | 35.96 | 7 |
| | ATOM | 1237 | CA | LYS | B | 420 | -14.278 | 69.609 | 25.538 | 1.00 | 40.82 | 6 |
| | ATOM | 1238 | CB | LYS | B | 420 | -14.452 | 68.103 | 25.271 | 1.00 | 40.78 | 6 |
| | ATOM | 1239 | CG | LYS | B | 420 | -13.349 | 67.214 | 25.830 | 1.00 | 48.62 | 6 |
| 10 | ATOM | 1240 | CD | LYS | B | 420 | -13.565 | 65.746 | 25.480 | 1.00 | 55.12 | 6 |
| | ATOM | 1241 | CE | LYS | B | 420 | -12.427 | 64.892 | 26.017 | 1.00 | 53.26 | 6 |
| | ATOM | 1242 | NZ | LYS | B | 420 | -12.582 | 63.457 | 25.608 | 1.00 | 52.69 | 7 |
| | ATOM | 1243 | C | LYS | B | 420 | -15.414 | 70.374 | 24.875 | 1.00 | 40.29 | 6 |
| | ATOM | 1244 | O | LYS | B | 420 | -15.225 | 71.015 | 23.851 | 1.00 | 39.66 | 8 |
| 15 | ATOM | 1245 | N | LEU | B | 421 | -16.591 | 70.300 | 25.499 | 1.00 | 38.33 | 7 |
| | ATOM | 1246 | CA | LEU | B | 421 | -17.796 | 70.958 | 25.001 | 1.00 | 37.60 | 6 |
| | ATOM | 1247 | CB | LEU | B | 421 | -18.970 | 70.702 | 25.965 | 1.00 | 43.66 | 6 |
| | ATOM | 1248 | CG | LEU | B | 421 | -20.370 | 70.850 | 25.418 | 1.00 | 46.50 | 6 |
| | ATOM | 1249 | CD1 | LEU | B | 421 | -20.529 | 69.890 | 24.255 | 1.00 | 45.15 | 6 |
| 20 | ATOM | 1250 | CD2 | LEU | B | 421 | -21.383 | 70.538 | 26.486 | 1.00 | 51.31 | 6 |
| | ATOM | 1251 | C | LEU | B | 421 | -17.547 | 72.452 | 24.823 | 1.00 | 39.59 | 6 |
| | ATOM | 1252 | O | LEU | B | 421 | -17.975 | 73.035 | 23.836 | 1.00 | 40.66 | 8 |
| | ATOM | 1253 | N | LEU | B | 422 | -16.847 | 73.059 | 25.780 | 1.00 | 39.57 | 7 |
| | ATOM | 1254 | CA | LEU | B | 422 | -16.534 | 74.478 | 25.715 | 1.00 | 38.63 | 6 |
| 25 | ATOM | 1255 | CB | LEU | B | 422 | -15.829 | 74.936 | 26.992 | 1.00 | 41.79 | 6 |
| | ATOM | 1256 | CG | LEU | B | 422 | -16.714 | 75.149 | 28.191 | 1.00 | 42.74 | 6 |
| | ATOM | 1257 | CD1 | LEU | B | 422 | -15.911 | 75.685 | 29.360 | 1.00 | 42.89 | 6 |
| | ATOM | 1258 | CD2 | LEU | B | 422 | -17.783 | 76.162 | 27.813 | 1.00 | 39.27 | 6 |
| | ATOM | 1259 | C | LEU | B | 422 | -15.677 | 74.788 | 24.513 | 1.00 | 40.47 | 6 |
| 30 | ATOM | 1260 | O | LEU | B | 422 | -15.823 | 75.846 | 23.917 | 1.00 | 47.83 | 8 |
| | ATOM | 1261 | N | MET | B | 423 | -14.789 | 73.853 | 24.168 | 1.00 | 34.27 | 7 |
| | ATOM | 1262 | CA | MET | B | 423 | -13.907 | 74.019 | 23.024 | 1.00 | 35.25 | 6 |
| | ATOM | 1263 | CB | MET | B | 423 | -12.920 | 72.858 | 22.922 | 1.00 | 32.56 | 6 |
| | ATOM | 1264 | CG | MET | B | 423 | -12.013 | 72.703 | 24.125 | 1.00 | 40.70 | 6 |
| 35 | ATOM | 1265 | SD | MET | B | 423 | -10.345 | 72.007 | 23.784 | 1.00 | 47.65 | 16 |
| | ATOM | 1266 | CE | MET | B | 423 | -10.770 | 70.538 | 22.761 | 1.00 | 47.16 | 6 |
| | ATOM | 1267 | C | MET | B | 423 | -14.709 | 74.100 | 21.738 | 1.00 | 35.13 | 6 |
| | ATOM | 1268 | O | MET | B | 423 | -14.341 | 74.807 | 20.803 | 1.00 | 29.85 | 8 |
| | ATOM | 1269 | N | LYS | B | 424 | -15.811 | 73.361 | 21.704 | 1.00 | 31.56 | 7 |
| 40 | ATOM | 1270 | CA | LYS | B | 424 | -16.676 | 73.354 | 20.544 | 1.00 | 32.29 | 6 |
| | ATOM | 1271 | CB | LYS | B | 424 | -17.783 | 72.316 | 20.736 | 1.00 | 30.56 | 6 |
| | ATOM | 1272 | CG | LYS | B | 424 | -17.257 | 70.879 | 20.843 | 1.00 | 30.07 | 6 |
| | ATOM | 1273 | CD | LYS | B | 424 | -16.444 | 70.510 | 19.611 | 1.00 | 33.22 | 6 |
| | ATOM | 1274 | CE | LYS | B | 424 | -15.795 | 69.136 | 19.706 | 1.00 | 28.75 | 6 |
| 45 | ATOM | 1275 | NZ | LYS | B | 424 | -14.655 | 69.067 | 20.678 | 1.00 | 31.01 | 7 |
| | ATOM | 1276 | C | LYS | B | 424 | -17.248 | 74.754 | 20.304 | 1.00 | 29.26 | 6 |
| | ATOM | 1277 | O | LYS | B | 424 | -17.439 | 75.149 | 19.166 | 1.00 | 30.22 | 8 |
| | ATOM | 1278 | N | VAL | B | 425 | -17.495 | 75.499 | 21.385 | 1.00 | 23.53 | 7 |
| | ATOM | 1279 | CA | VAL | B | 425 | -18.014 | 76.852 | 21.278 | 1.00 | 28.91 | 6 |
| 50 | ATOM | 1280 | CB | VAL | B | 425 | -18.278 | 77.458 | 22.663 | 1.00 | 29.44 | 6 |
| | ATOM | 1281 | CG1 | VAL | B | 425 | -18.633 | 78.915 | 22.547 | 1.00 | 28.81 | 6 |
| | ATOM | 1282 | CG2 | VAL | B | 425 | -19.401 | 76.733 | 23.354 | 1.00 | 31.22 | 6 |
| | ATOM | 1283 | C | VAL | B | 425 | -17.001 | 77.682 | 20.498 | 1.00 | 32.03 | 6 |
| | ATOM | 1284 | O | VAL | B | 425 | -17.368 | 78.465 | 19.629 | 1.00 | 31.95 | 8 |
| 55 | ATOM | 1285 | N | THR | B | 426 | -15.721 | 77.508 | 20.827 | 1.00 | 33.61 | 7 |
| | ATOM | 1286 | CA | THR | B | 426 | -14.645 | 78.221 | 20.137 | 1.00 | 30.76 | 6 |
| | ATOM | 1287 | CB | THR | B | 426 | -13.270 | 77.912 | 20.761 | 1.00 | 32.34 | 6 |
| | ATOM | 1288 | OG1 | THR | B | 426 | -13.073 | 78.697 | 21.941 | 1.00 | 33.07 | 8 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 1289 | CG2 | THR | B | 426 | -12.153 | 78.174 | 19.782 | 1.00 | 25.40 | 6 |
| | ATOM | 1290 | C | THR | B | 426 | -14.677 | 77.742 | 18.706 | 1.00 | 32.53 | 6 |
| | ATOM | 1291 | O | THR | B | 426 | -14.639 | 78.530 | 17.763 | 1.00 | 35.19 | 8 |
| | ATOM | 1292 | N | ASP | B | 427 | -14.749 | 76.425 | 18.566 | 1.00 | 28.83 | 7 |
| | ATOM | 1293 | CA | ASP | B | 427 | -14.796 | 75.807 | 17.257 | 1.00 | 35.12 | 6 |
| 10 | ATOM | 1294 | CB | ASP | B | 427 | -15.096 | 74.302 | 17.380 | 1.00 | 39.14 | 6 |
| | ATOM | 1295 | CG | ASP | B | 427 | -13.910 | 73.496 | 17.806 | 1.00 | 45.80 | 6 |
| | ATOM | 1296 | OD1 | ASP | B | 427 | -12.786 | 73.774 | 17.348 | 1.00 | 41.97 | 8 |
| | ATOM | 1297 | OD2 | ASP | B | 427 | -14.064 | 72.517 | 18.583 | 1.00 | 50.06 | 8 |
| | ATOM | 1298 | C | ASP | B | 427 | -15.883 | 76.502 | 16.429 | 1.00 | 33.94 | 6 |
| 15 | ATOM | 1299 | O | ASP | B | 427 | -15.673 | 76.815 | 15.262 | 1.00 | 38.02 | 8 |
| | ATOM | 1300 | N | LEU | B | 428 | -17.040 | 76.741 | 17.048 | 1.00 | 27.15 | 7 |
| | ATOM | 1301 | CA | LEU | B | 428 | -18.154 | 77.388 | 16.367 | 1.00 | 29.99 | 6 |
| | ATOM | 1302 | CB | LEU | B | 428 | -19.448 | 77.190 | 17.168 | 1.00 | 22.49 | 6 |
| | ATOM | 1303 | CG | LEU | B | 428 | -20.086 | 75.818 | 17.089 | 1.00 | 25.54 | 6 |
| 20 | ATOM | 1304 | CD1 | LEU | B | 428 | -21.282 | 75.729 | 18.012 | 1.00 | 20.60 | 6 |
| | ATOM | 1305 | CD2 | LEU | B | 428 | -20.509 | 75.564 | 15.651 | 1.00 | 17.24 | 6 |
| | ATOM | 1306 | C | LEU | B | 428 | -17.901 | 78.863 | 16.103 | 1.00 | 28.94 | 6 |
| | ATOM | 1307 | O | LEU | B | 428 | -18.328 | 79.388 | 15.076 | 1.00 | 31.26 | 8 |
| | ATOM | 1308 | N | ARG | B | 429 | -17.213 | 79.524 | 17.035 | 1.00 | 27.64 | 7 |
| 25 | ATOM | 1309 | CA | ARG | B | 429 | -16.894 | 80.937 | 16.883 | 1.00 | 28.13 | 6 |
| | ATOM | 1310 | CB | ARG | B | 429 | -16.274 | 81.507 | 18.160 | 1.00 | 29.59 | 6 |
| | ATOM | 1311 | CG | ARG | B | 429 | -17.246 | 81.752 | 19.302 | 1.00 | 34.85 | 6 |
| | ATOM | 1312 | CD | ARG | B | 429 | -16.626 | 82.653 | 20.372 | 1.00 | 47.18 | 6 |
| | ATOM | 1313 | NE | ARG | B | 429 | -17.373 | 82.714 | 21.620 | 1.00 | 57.93 | 7 |
| 30 | ATOM | 1314 | CZ | ARG | B | 429 | -18.632 | 83.124 | 21.716 | 1.00 | 63.62 | 6 |
| | ATOM | 1315 | NH1 | ARG | B | 429 | -19.263 | 83.579 | 20.622 | 1.00 | 60.71 | 7 |
| | ATOM | 1316 | NH2 | ARG | B | 429 | -19.238 | 83.130 | 22.916 | 1.00 | 62.38 | 7 |
| | ATOM | 1317 | C | ARG | B | 429 | -15.930 | 81.146 | 15.728 | 1.00 | 29.81 | 6 |
| | ATOM | 1318 | O | ARG | B | 429 | -16.101 | 82.061 | 14.933 | 1.00 | 30.81 | 8 |
| 35 | ATOM | 1319 | N | MET | B | 430 | -14.908 | 80.295 | 15.670 | 1.00 | 29.64 | 7 |
| | ATOM | 1320 | CA | MET | B | 430 | -13.920 | 80.343 | 14.614 | 1.00 | 34.72 | 6 |
| | ATOM | 1321 | CB | MET | B | 430 | -12.939 | 79.192 | 14.763 | 1.00 | 34.97 | 6 |
| | ATOM | 1322 | CG | MET | B | 430 | -11.787 | 79.431 | 15.689 | 1.00 | 45.34 | 6 |
| | ATOM | 1323 | SD | MET | B | 430 | -10.729 | 80.768 | 15.158 | 1.00 | 52.55 | 16 |
| 40 | ATOM | 1324 | CE | MET | B | 430 | -10.070 | 80.157 | 13.610 | 1.00 | 55.56 | 6 |
| | ATOM | 1325 | C | MET | B | 430 | -14.638 | 80.217 | 13.284 | 1.00 | 34.01 | 6 |
| | ATOM | 1326 | O | MET | B | 430 | -14.395 | 80.996 | 12.385 | 1.00 | 37.29 | 8 |
| | ATOM | 1327 | N | ILE | B | 431 | -15.516 | 79.217 | 13.176 | 1.00 | 29.99 | 7 |
| | ATOM | 1328 | CA | ILE | B | 431 | -16.296 | 78.992 | 11.963 | 1.00 | 28.82 | 6 |
| 45 | ATOM | 1329 | CB | ILE | B | 431 | -17.391 | 77.929 | 12.177 | 1.00 | 27.39 | 6 |
| | ATOM | 1330 | CG2 | ILE | B | 431 | -18.314 | 77.841 | 10.959 | 1.00 | 23.87 | 6 |
| | ATOM | 1331 | CG1 | ILE | B | 431 | -16.784 | 76.555 | 12.449 | 1.00 | 25.56 | 6 |
| | ATOM | 1332 | CD1 | ILE | B | 431 | -17.826 | 75.464 | 12.498 | 1.00 | 17.29 | 6 |
| | ATOM | 1333 | C | ILE | B | 431 | -16.953 | 80.288 | 11.538 | 1.00 | 29.49 | 6 |
| 50 | ATOM | 1334 | O | ILE | B | 431 | -16.837 | 80.725 | 10.398 | 1.00 | 24.19 | 8 |
| | ATOM | 1335 | N | GLY | B | 432 | -17.657 | 80.904 | 12.474 | 1.00 | 25.25 | 7 |
| | ATOM | 1336 | CA | GLY | B | 432 | -18.357 | 82.142 | 12.179 | 1.00 | 30.38 | 6 |
| | ATOM | 1337 | C | GLY | B | 432 | -17.395 | 83.209 | 11.725 | 1.00 | 32.75 | 6 |
| | ATOM | 1338 | O | GLY | B | 432 | -17.531 | 83.740 | 10.637 | 1.00 | 36.38 | 8 |
| 55 | ATOM | 1339 | N | ALA | B | 433 | -16.431 | 83.522 | 12.586 | 1.00 | 26.77 | 7 |
| | ATOM | 1340 | CA | ALA | B | 433 | -15.407 | 84.514 | 12.299 | 1.00 | 26.48 | 6 |
| | ATOM | 1341 | CB | ALA | B | 433 | -14.240 | 84.338 | 13.253 | 1.00 | 19.90 | 6 |
| | ATOM | 1342 | C | ALA | B | 433 | -14.905 | 84.433 | 10.867 | 1.00 | 30.73 | 6 |

| | | | | | | | | | | |
|----|------|------|-----|-----------|---------|--------|--------|------|-------|----|
| 5 | ATOM | 1343 | O | ALA B 433 | -14.849 | 85.432 | 10.171 | 1.00 | 31.60 | 8 |
| | ATOM | 1344 | N | CYS B 434 | -14.534 | 83.246 | 10.439 | 1.00 | 33.22 | 7 |
| | ATOM | 1345 | CA | CYS B 434 | -14.023 | 83.021 | 9.120 | 1.00 | 34.34 | 6 |
| | ATOM | 1346 | CB | CYS B 434 | -13.553 | 81.661 | 9.226 | 1.00 | 35.20 | 6 |
| | ATOM | 1347 | SG | CYS B 434 | -12.412 | 81.249 | 8.444 | 1.00 | 54.48 | 16 |
| 10 | ATOM | 1348 | C | CYS B 434 | -15.106 | 83.116 | 8.062 | 1.00 | 34.09 | 6 |
| | ATOM | 1349 | O | CYS B 434 | -14.844 | 83.555 | 6.952 | 1.00 | 34.89 | 8 |
| | ATOM | 1350 | N | HIS B 435 | -16.318 | 82.699 | 8.394 | 1.00 | 34.30 | 7 |
| | ATOM | 1351 | CA | HIS B 435 | -17.395 | 82.762 | 7.443 | 1.00 | 35.44 | 6 |
| | ATOM | 1352 | CB | HIS B 435 | -18.700 | 82.404 | 8.103 | 1.00 | 31.76 | 6 |
| 15 | ATOM | 1353 | CG | HIS B 435 | -19.845 | 82.425 | 7.149 | 1.00 | 32.03 | 6 |
| | ATOM | 1354 | CD2 | HIS B 435 | -20.483 | 81.419 | 6.515 | 1.00 | 28.61 | 6 |
| | ATOM | 1355 | ND1 | HIS B 435 | -20.345 | 83.600 | 6.607 | 1.00 | 28.48 | 7 |
| | ATOM | 1356 | CE1 | HIS B 435 | -21.241 | 83.293 | 5.672 | 1.00 | 33.27 | 6 |
| | ATOM | 1357 | NE2 | HIS B 435 | -21.341 | 81.977 | 5.605 | 1.00 | 31.57 | 7 |
| 20 | ATOM | 1358 | C | HIS B 435 | -17.528 | 84.152 | 6.878 | 1.00 | 32.74 | 6 |
| | ATOM | 1359 | O | HIS B 435 | -17.842 | 84.326 | 5.715 | 1.00 | 32.87 | 8 |
| | ATOM | 1360 | N | ALA B 436 | -17.315 | 85.121 | 7.758 | 1.00 | 31.01 | 7 |
| | ATOM | 1361 | CA | ALA B 436 | -17.376 | 86.520 | 7.405 | 1.00 | 29.91 | 6 |
| | ATOM | 1362 | CB | ALA B 436 | -17.008 | 87.352 | 8.618 | 1.00 | 21.23 | 6 |
| 25 | ATOM | 1363 | C | ALA B 436 | -16.393 | 86.782 | 6.266 | 1.00 | 33.86 | 6 |
| | ATOM | 1364 | O | ALA B 436 | -16.734 | 87.398 | 5.257 | 1.00 | 36.10 | 8 |
| | ATOM | 1365 | N | SER B 437 | -15.162 | 86.307 | 6.448 | 1.00 | 35.19 | 7 |
| | ATOM | 1366 | CA | SER B 437 | -14.122 | 86.484 | 5.445 | 1.00 | 33.03 | 6 |
| | ATOM | 1367 | CB | SER B 437 | -12.882 | 85.688 | 5.847 | 1.00 | 35.31 | 6 |
| 30 | ATOM | 1368 | OG | SER B 437 | -11.855 | 85.824 | 4.879 | 1.00 | 44.99 | 8 |
| | ATOM | 1369 | C | SER B 437 | -14.642 | 85.993 | 4.108 | 1.00 | 38.39 | 6 |
| | ATOM | 1370 | O | SER B 437 | -14.700 | 86.730 | 3.127 | 1.00 | 37.54 | 8 |
| | ATOM | 1371 | N | ARG B 438 | -15.008 | 84.719 | 4.096 | 1.00 | 37.32 | 7 |
| | ATOM | 1372 | CA | ARG B 438 | -15.526 | 84.068 | 2.908 | 1.00 | 39.30 | 6 |
| 35 | ATOM | 1373 | CB | ARG B 438 | -16.019 | 82.660 | 3.259 | 1.00 | 42.97 | 6 |
| | ATOM | 1374 | CG | ARG B 438 | -14.910 | 81.673 | 3.590 | 1.00 | 41.72 | 6 |
| | ATOM | 1375 | CD | ARG B 438 | -14.044 | 81.488 | 2.356 | 1.00 | 45.23 | 6 |
| | ATOM | 1376 | NE | ARG B 438 | -14.781 | 80.936 | 1.235 | 1.00 | 45.66 | 7 |
| | ATOM | 1377 | CZ | ARG B 438 | -14.482 | 81.175 | -0.040 | 1.00 | 49.71 | 6 |
| 40 | ATOM | 1378 | NH1 | ARG B 438 | -13.458 | 81.977 | -0.347 | 1.00 | 50.91 | 7 |
| | ATOM | 1379 | NH2 | ARG B 438 | -15.219 | 80.619 | -1.002 | 1.00 | 46.86 | 7 |
| | ATOM | 1380 | C | ARG B 438 | -16.659 | 84.859 | 2.287 | 1.00 | 42.37 | 6 |
| | ATOM | 1381 | O | ARG B 438 | -16.841 | 84.832 | 1.072 | 1.00 | 40.58 | 8 |
| | ATOM | 1382 | N | PHE B 439 | -17.417 | 85.575 | 3.117 | 1.00 | 42.25 | 7 |
| 45 | ATOM | 1383 | CA | PHE B 439 | -18.531 | 86.354 | 2.614 | 1.00 | 42.81 | 6 |
| | ATOM | 1384 | CB | PHE B 439 | -19.198 | 87.132 | 3.731 | 1.00 | 42.18 | 6 |
| | ATOM | 1385 | CG | PHE B 439 | -20.487 | 87.769 | 3.323 | 1.00 | 42.48 | 6 |
| | ATOM | 1386 | CD1 | PHE B 439 | -21.535 | 86.981 | 2.912 | 1.00 | 47.09 | 6 |
| | ATOM | 1387 | CD2 | PHE B 439 | -20.638 | 89.141 | 3.334 | 1.00 | 39.76 | 6 |
| 50 | ATOM | 1388 | CE1 | PHE B 439 | -22.735 | 87.543 | 2.527 | 1.00 | 49.17 | 6 |
| | ATOM | 1389 | CE2 | PHE B 439 | -21.851 | 89.717 | 2.944 | 1.00 | 45.10 | 6 |
| | ATOM | 1390 | CZ | PHE B 439 | -22.901 | 88.911 | 2.538 | 1.00 | 46.36 | 6 |
| | ATOM | 1391 | C | PHE B 439 | -18.016 | 87.319 | 1.581 | 1.00 | 44.79 | 6 |
| | ATOM | 1392 | O | PHE B 439 | -18.514 | 87.354 | 0.465 | 1.00 | 40.26 | 8 |
| 55 | ATOM | 1393 | N | LEU B 440 | -17.021 | 88.117 | 1.987 | 1.00 | 42.77 | 7 |
| | ATOM | 1394 | CA | LEU B 440 | -16.415 | 89.115 | 1.109 | 1.00 | 42.96 | 6 |
| | ATOM | 1395 | CB | LEU B 440 | -15.169 | 89.718 | 1.768 | 1.00 | 37.19 | 6 |
| | ATOM | 1396 | CG | LEU B 440 | -15.477 | 90.588 | 2.967 | 1.00 | 36.97 | 6 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 1397 | CD1 | LEU | B | 440 | -14.219 | 91.886 | 3.402 | 1.00 | 33.65 | 6 |
| | ATOM | 1398 | CD2 | LEU | B | 440 | -16.577 | 91.591 | 2.574 | 1.00 | 35.42 | 6 |
| | ATOM | 1399 | C | LEU | B | 440 | -16.099 | 88.561 | -0.273 | 1.00 | 45.47 | 6 |
| | ATOM | 1400 | O | LEU | B | 440 | -16.631 | 89.059 | -1.265 | 1.00 | 52.48 | 8 |
| | ATOM | 1401 | N | HIS | B | 441 | -15.238 | 87.549 | -0.345 | 1.00 | 49.15 | 7 |
| 10 | ATOM | 1402 | CA | HIS | B | 441 | -14.929 | 86.956 | -1.632 | 1.00 | 54.76 | 6 |
| | ATOM | 1403 | CB | HIS | B | 441 | -14.150 | 85.700 | -1.448 | 1.00 | 56.68 | 6 |
| | ATOM | 1404 | CG | HIS | B | 441 | -12.713 | 85.934 | -1.230 | 1.00 | 62.73 | 6 |
| | ATOM | 1405 | CD2 | HIS | B | 441 | -11.602 | 85.418 | -1.812 | 1.00 | 65.73 | 6 |
| | ATOM | 1406 | ND1 | HIS | B | 441 | -12.245 | 86.850 | -0.273 | 1.00 | 66.01 | 7 |
| 15 | ATOM | 1407 | CE1 | HIS | B | 441 | -10.916 | 86.847 | -0.309 | 1.00 | 65.55 | 6 |
| | ATOM | 1408 | NE2 | HIS | B | 441 | -10.512 | 85.993 | -1.228 | 1.00 | 60.09 | 7 |
| | ATOM | 1409 | C | HIS | B | 441 | -16.217 | 86.633 | -2.301 | 1.00 | 55.93 | 6 |
| | ATOM | 1410 | O | HIS | B | 441 | -16.418 | 86.938 | -3.465 | 1.00 | 57.33 | 8 |
| | ATOM | 1411 | N | MET | B | 442 | -17.106 | 85.997 | -1.553 | 1.00 | 57.81 | 7 |
| 20 | ATOM | 1412 | CA | MET | B | 442 | -18.399 | 85.652 | -2.106 | 1.00 | 59.11 | 6 |
| | ATOM | 1413 | CB | MET | B | 442 | -19.340 | 85.162 | -1.008 | 1.00 | 55.93 | 6 |
| | ATOM | 1414 | CG | MET | B | 442 | -18.991 | 83.796 | -0.456 | 1.00 | 58.52 | 6 |
| | ATOM | 1415 | SD | MET | B | 442 | -20.310 | 82.994 | 0.505 | 1.00 | 60.99 | 16 |
| | ATOM | 1416 | CE | MET | B | 442 | -20.525 | 84.203 | 1.827 | 1.00 | 52.61 | 6 |
| 25 | ATOM | 1417 | C | MET | B | 442 | -18.991 | 86.879 | -2.785 | 1.00 | 60.31 | 6 |
| | ATOM | 1418 | O | MET | B | 442 | -19.646 | 86.778 | -3.817 | 1.00 | 58.18 | 8 |
| | ATOM | 1419 | N | LYS | B | 443 | -18.731 | 88.045 | -2.213 | 1.00 | 61.45 | 7 |
| | ATOM | 1420 | CA | LYS | B | 443 | -19.267 | 89.268 | -2.758 | 1.00 | 64.90 | 6 |
| | ATOM | 1421 | CB | LYS | B | 443 | -19.182 | 90.358 | -1.704 | 1.00 | 64.40 | 6 |
| 30 | ATOM | 1422 | CG | LYS | B | 443 | -20.160 | 91.449 | -1.982 | 1.00 | 69.12 | 6 |
| | ATOM | 1423 | CD | LYS | B | 443 | -19.763 | 92.673 | -1.306 | 1.00 | 71.14 | 6 |
| | ATOM | 1424 | CE | LYS | B | 443 | -20.508 | 92.993 | -0.491 | 1.00 | 73.43 | 6 |
| | ATOM | 1425 | NZ | LYS | B | 443 | -20.174 | 94.242 | 0.151 | 1.00 | 67.97 | 7 |
| | ATOM | 1426 | C | LYS | B | 443 | -18.528 | 89.704 | -4.020 | 1.00 | 67.29 | 6 |
| 35 | ATOM | 1427 | O | LYS | B | 443 | -18.979 | 90.586 | -4.731 | 1.00 | 67.90 | 8 |
| | ATOM | 1428 | N | VAL | B | 444 | -17.383 | 89.075 | -4.285 | 1.00 | 66.57 | 7 |
| | ATOM | 1429 | CA | VAL | B | 444 | -16.589 | 89.418 | -5.455 | 1.00 | 64.76 | 6 |
| | ATOM | 1430 | CB | VAL | B | 444 | -15.097 | 89.568 | -5.082 | 1.00 | 62.76 | 6 |
| | ATOM | 1431 | CG1 | VAL | B | 444 | -14.269 | 89.857 | -6.298 | 1.00 | 64.00 | 6 |
| 40 | ATOM | 1432 | CG2 | VAL | B | 444 | -14.905 | 90.678 | -4.042 | 1.00 | 59.27 | 6 |
| | ATOM | 1433 | C | VAL | B | 444 | -16.800 | 88.397 | -6.569 | 1.00 | 68.61 | 6 |
| | ATOM | 1434 | O | VAL | B | 444 | -16.968 | 88.774 | -7.729 | 1.00 | 70.60 | 8 |
| | ATOM | 1435 | N | GLU | B | 445 | -16.812 | 87.118 | -6.219 | 1.00 | 70.71 | 7 |
| | ATOM | 1436 | CA | GLU | B | 445 | -16.951 | 86.033 | -7.197 | 1.00 | 71.45 | 6 |
| 45 | ATOM | 1437 | CB | GLU | B | 445 | -16.169 | 84.809 | -6.712 | 1.00 | 72.36 | 6 |
| | ATOM | 1438 | CG | GLU | B | 445 | -14.736 | 85.090 | -6.392 | 1.00 | 40.00 | 6 |
| | ATOM | 1439 | CD | GLU | B | 445 | -13.998 | 83.890 | -5.851 | 1.00 | 40.00 | 6 |
| | ATOM | 1440 | OE1 | GLU | B | 445 | -14.587 | 82.798 | -5.665 | 1.00 | 40.00 | 8 |
| | ATOM | 1441 | OE2 | GLU | B | 445 | -12.775 | 83.995 | -5.580 | 1.00 | 40.00 | 8 |
| 50 | ATOM | 1442 | C | GLU | B | 445 | -18.375 | 85.574 | -7.422 | 1.00 | 71.46 | 6 |
| | ATOM | 1443 | O | GLU | B | 445 | -18.605 | 84.542 | -8.064 | 1.00 | 73.02 | 8 |
| | ATOM | 1444 | N | CYS | B | 446 | -19.328 | 86.333 | -6.900 | 1.00 | 71.12 | 7 |
| | ATOM | 1445 | CA | CYS | B | 446 | -20.694 | 85.942 | -7.062 | 1.00 | 70.83 | 6 |
| | ATOM | 1446 | CB | CYS | B | 446 | -21.196 | 85.230 | -5.784 | 1.00 | 71.05 | 6 |
| 55 | ATOM | 1447 | SG | CYS | B | 446 | -20.296 | 83.720 | -5.349 | 1.00 | 72.83 | 16 |
| | ATOM | 1448 | C | CYS | B | 446 | -21.563 | 87.135 | -7.386 | 1.00 | 71.91 | 6 |
| | ATOM | 1449 | O | CYS | B | 446 | -21.307 | 88.244 | -6.911 | 1.00 | 72.06 | 8 |
| | ATOM | 1450 | N | PRO | B | 447 | -22.550 | 86.928 | -8.256 | 1.00 | 73.12 | 7 |

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|----|------|------|-----|-----------|---------|--------|---------|------|-------|---|
| 5 | ATOM | 1451 | CD | PRO B 447 | -22.837 | 85.637 | -8.886 | 1.00 | 72.88 | 6 |
| | ATOM | 1452 | CA | PRO B 447 | -23.461 | 87.997 | -8.653 | 1.00 | 74.22 | 6 |
| | ATOM | 1453 | CB | PRO B 447 | -24.399 | 87.338 | -9.659 | 1.00 | 72.98 | 6 |
| | ATOM | 1454 | CG | PRO B 447 | -23.981 | 85.934 | -9.776 | 1.00 | 74.77 | 6 |
| | ATOM | 1455 | C | PRO B 447 | -24.203 | 88.519 | -7.451 | 1.00 | 75.94 | 6 |
| 10 | ATOM | 1456 | O | PRO B 447 | -24.601 | 87.749 | -6.611 | 1.00 | 76.67 | 8 |
| | ATOM | 1457 | N | THR B 448 | -24.390 | 89.828 | -7.373 | 1.00 | 76.91 | 7 |
| | ATOM | 1458 | CA | THR B 448 | -25.134 | 90.436 | -6.268 | 1.00 | 78.24 | 6 |
| | ATOM | 1459 | CB | THR B 448 | -24.883 | 91.948 | -6.276 | 1.00 | 81.33 | 6 |
| | ATOM | 1460 | OG1 | THR B 448 | -25.474 | 92.525 | -7.451 | 1.00 | 84.46 | 8 |
| 15 | ATOM | 1461 | CG2 | THR B 448 | -23.394 | 92.234 | -6.269 | 1.00 | 83.51 | 6 |
| | ATOM | 1462 | C | THR B 448 | -26.594 | 90.160 | -6.619 | 1.00 | 77.42 | 6 |
| | ATOM | 1463 | O | THR B 448 | -27.512 | 90.649 | -5.982 | 1.00 | 77.65 | 8 |
| | ATOM | 1464 | N | GLU B 449 | -26.759 | 89.400 | -7.697 | 1.00 | 76.29 | 7 |
| | ATOM | 1465 | CA | GLU B 449 | -28.051 | 89.017 | -8.211 | 1.00 | 75.03 | 6 |
| 20 | ATOM | 1466 | CB | GLU B 449 | -27.923 | 88.915 | -9.719 | 1.00 | 74.62 | 6 |
| | ATOM | 1467 | CG | GLU B 449 | -28.823 | 87.966 | -10.343 | 1.00 | 40.00 | 6 |
| | ATOM | 1468 | CD | GLU B 449 | -28.522 | 87.831 | -11.756 | 1.00 | 40.00 | 6 |
| | ATOM | 1469 | OE1 | GLU B 449 | -27.366 | 88.072 | -12.190 | 1.00 | 40.00 | 8 |
| | ATOM | 1470 | OE2 | GLU B 449 | -29.449 | 87.438 | -12.492 | 1.00 | 40.00 | 8 |
| 25 | ATOM | 1471 | C | GLU B 449 | -28.448 | 87.660 | -7.609 | 1.00 | 73.49 | 6 |
| | ATOM | 1472 | O | GLU B 449 | -29.479 | 87.092 | -7.953 | 1.00 | 70.24 | 8 |
| | ATOM | 1473 | N | LEU B 450 | -27.624 | 87.158 | -6.695 | 1.00 | 70.80 | 7 |
| | ATOM | 1474 | CA | LEU B 450 | -27.879 | 85.879 | -6.058 | 1.00 | 68.82 | 6 |
| | ATOM | 1475 | CB | LEU B 450 | -26.772 | 84.887 | -6.447 | 1.00 | 71.91 | 6 |
| 30 | ATOM | 1476 | CG | LEU B 450 | -26.612 | 84.503 | -7.900 | 1.00 | 76.62 | 6 |
| | ATOM | 1477 | CD1 | LEU B 450 | -25.396 | 83.637 | -8.059 | 1.00 | 77.95 | 6 |
| | ATOM | 1478 | CD2 | LEU B 450 | -27.849 | 83.775 | -8.351 | 1.00 | 76.46 | 6 |
| | ATOM | 1479 | C | LEU B 450 | -27.941 | 86.012 | -4.536 | 1.00 | 66.22 | 6 |
| | ATOM | 1480 | O | LEU B 450 | -28.251 | 85.039 | -3.849 | 1.00 | 66.01 | 8 |
| 35 | ATOM | 1481 | N | PHE B 451 | -27.666 | 87.215 | -4.012 | 1.00 | 61.96 | 7 |
| | ATOM | 1482 | CA | PHE B 451 | -27.635 | 87.494 | -2.585 | 1.00 | 58.44 | 6 |
| | ATOM | 1483 | CB | PHE B 451 | -26.579 | 88.573 | -2.263 | 1.00 | 61.34 | 6 |
| | ATOM | 1484 | CG | PHE B 451 | -25.153 | 88.078 | -2.413 | 1.00 | 63.02 | 6 |
| | ATOM | 1485 | CD1 | PHE B 451 | -24.675 | 87.587 | -3.626 | 1.00 | 62.92 | 6 |
| 40 | ATOM | 1486 | CD2 | PHE B 451 | -24.283 | 88.173 | -1.346 | 1.00 | 63.07 | 6 |
| | ATOM | 1487 | CE1 | PHE B 451 | -23.327 | 87.217 | -3.757 | 1.00 | 65.12 | 6 |
| | ATOM | 1488 | CE2 | PHE B 451 | -22.939 | 87.806 | -1.472 | 1.00 | 64.66 | 6 |
| | ATOM | 1489 | CZ | PHE B 451 | -22.459 | 87.335 | -2.686 | 1.00 | 67.12 | 6 |
| | ATOM | 1490 | C | PHE B 451 | -28.931 | 87.994 | -1.962 | 1.00 | 56.41 | 6 |
| 45 | ATOM | 1491 | O | PHE B 451 | -29.207 | 89.214 | -1.908 | 1.00 | 56.56 | 8 |
| | ATOM | 1492 | N | PRO B 452 | -29.791 | 87.072 | -1.473 | 1.00 | 53.28 | 7 |
| | ATOM | 1493 | CD | PRO B 452 | -29.767 | 85.611 | -1.494 | 1.00 | 50.46 | 6 |
| | ATOM | 1494 | CA | PRO B 452 | -31.037 | 87.598 | -0.843 | 1.00 | 50.26 | 6 |
| | ATOM | 1495 | CB | PRO B 452 | -31.746 | 86.375 | -0.301 | 1.00 | 49.19 | 6 |
| 50 | ATOM | 1496 | CG | PRO B 452 | -31.024 | 85.197 | -0.842 | 1.00 | 45.89 | 6 |
| | ATOM | 1497 | C | PRO B 452 | -30.636 | 88.567 | 0.251 | 1.00 | 49.62 | 6 |
| | ATOM | 1498 | O | PRO B 452 | -29.628 | 88.401 | 0.906 | 1.00 | 52.35 | 8 |
| | ATOM | 1499 | N | PRO B 453 | -31.494 | 89.539 | 0.535 | 1.00 | 51.50 | 7 |
| | ATOM | 1500 | CD | PRO B 453 | -32.853 | 89.644 | 0.022 | 1.00 | 49.66 | 6 |
| 55 | ATOM | 1501 | CA | PRO B 453 | -31.184 | 90.573 | 1.530 | 1.00 | 50.89 | 6 |
| | ATOM | 1502 | CB | PRO B 453 | -32.422 | 91.401 | 1.625 | 1.00 | 51.49 | 6 |
| | ATOM | 1503 | CG | PRO B 453 | -33.378 | 90.827 | 0.724 | 1.00 | 50.82 | 6 |
| | ATOM | 1504 | C | PRO B 453 | -30.829 | 90.039 | 2.906 | 1.00 | 50.99 | 6 |

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|----|------|------|-----|-----------|---------|--------|--------|------|-------|---|
| 5 | ATOM | 1505 | O | PRO B 453 | -29.700 | 90.206 | 3.345 | 1.00 | 54.17 | 8 |
| | ATOM | 1506 | N | LEU B 454 | -31.807 | 89.458 | 3.631 | 1.00 | 51.21 | 7 |
| | ATOM | 1507 | CA | LEU B 454 | -31.538 | 88.945 | 4.948 | 1.00 | 47.17 | 6 |
| | ATOM | 1508 | CB | LEU B 454 | -32.550 | 87.858 | 5.330 | 1.00 | 44.44 | 6 |
| | ATOM | 1509 | CG | LEU B 454 | -32.347 | 87.412 | 6.748 | 1.00 | 41.33 | 6 |
| 10 | ATOM | 1510 | CD1 | LEU B 454 | -31.987 | 88.589 | 7.631 | 1.00 | 35.93 | 6 |
| | ATOM | 1511 | CD2 | LEU B 454 | -33.590 | 86.732 | 7.239 | 1.00 | 34.79 | 6 |
| | ATOM | 1512 | C | LEU B 454 | -30.099 | 88.443 | 4.928 | 1.00 | 42.25 | 6 |
| | ATOM | 1513 | O | LEU B 454 | -29.323 | 88.774 | 5.812 | 1.00 | 40.82 | 8 |
| | ATOM | 1514 | N | PHE B 455 | -29.716 | 87.707 | 3.885 | 1.00 | 39.29 | 7 |
| 15 | ATOM | 1515 | CA | PHE B 455 | -28.347 | 87.204 | 3.770 | 1.00 | 41.81 | 6 |
| | ATOM | 1516 | CB | PHE B 455 | -28.132 | 86.536 | 2.418 | 1.00 | 47.22 | 6 |
| | ATOM | 1517 | CG | PHE B 455 | -26.813 | 85.836 | 2.292 | 1.00 | 56.97 | 6 |
| | ATOM | 1518 | CD1 | PHE B 455 | -26.437 | 84.915 | 3.247 | 1.00 | 57.23 | 6 |
| | ATOM | 1519 | CD2 | PHE B 455 | -25.949 | 86.094 | 1.236 | 1.00 | 59.40 | 6 |
| 20 | ATOM | 1520 | CE1 | PHE B 455 | -25.225 | 84.234 | 3.153 | 1.00 | 56.58 | 6 |
| | ATOM | 1521 | CE2 | PHE B 455 | -24.720 | 85.409 | 1.134 | 1.00 | 61.80 | 6 |
| | ATOM | 1522 | CZ | PHE B 455 | -24.360 | 84.481 | 2.103 | 1.00 | 59.94 | 6 |
| | ATOM | 1523 | C | PHE B 455 | -27.400 | 88.386 | 3.923 | 1.00 | 45.12 | 6 |
| | ATOM | 1524 | O | PHE B 455 | -26.657 | 88.450 | 4.889 | 1.00 | 39.95 | 8 |
| 25 | ATOM | 1525 | N | LEU B 456 | -27.439 | 89.303 | 2.949 | 1.00 | 43.92 | 7 |
| | ATOM | 1526 | CA | LEU B 456 | -26.597 | 90.503 | 2.947 | 1.00 | 44.08 | 6 |
| | ATOM | 1527 | CB | LEU B 456 | -27.001 | 91.440 | 1.802 | 1.00 | 50.20 | 6 |
| | ATOM | 1528 | CG | LEU B 456 | -26.439 | 91.155 | 0.432 | 1.00 | 55.79 | 6 |
| | ATOM | 1529 | CD1 | LEU B 456 | -27.064 | 92.082 | -0.591 | 1.00 | 54.70 | 6 |
| 30 | ATOM | 1530 | CD2 | LEU B 456 | -24.920 | 91.345 | 0.494 | 1.00 | 53.01 | 6 |
| | ATOM | 1531 | C | LEU B 456 | -26.689 | 91.245 | 4.264 | 1.00 | 44.65 | 6 |
| | ATOM | 1532 | O | LEU B 456 | -25.678 | 91.540 | 4.886 | 1.00 | 45.93 | 8 |
| | ATOM | 1533 | N | GLU B 457 | -27.990 | 91.268 | 4.265 | 1.00 | 44.56 | 7 |
| | ATOM | 1534 | CA | GLU B 457 | -28.288 | 92.016 | 5.497 | 1.00 | 46.37 | 6 |
| 35 | ATOM | 1535 | C | GLU B 457 | -27.434 | 91.452 | 6.628 | 1.00 | 43.60 | 6 |
| | ATOM | 1536 | O | GLU B 457 | -26.754 | 92.223 | 7.339 | 1.00 | 42.69 | 8 |
| | ATOM | 1537 | CB | GLU B 457 | -29.769 | 91.879 | 5.855 | 1.00 | 50.16 | 6 |
| | ATOM | 1538 | CG | GLU B 457 | -30.208 | 92.849 | 6.954 | 1.00 | 20.00 | 6 |
| | ATOM | 1539 | CD | GLU B 457 | -31.646 | 93.338 | 6.782 | 1.00 | 20.00 | 6 |
| 40 | ATOM | 1540 | OE1 | GLU B 457 | -32.351 | 92.932 | 5.779 | 1.00 | 20.00 | 8 |
| | ATOM | 1541 | OE2 | GLU B 457 | -32.157 | 94.156 | 7.638 | 1.00 | 20.00 | 8 |
| | ATOM | 1542 | N | VAL B 458 | -27.428 | 90.413 | 7.281 | 1.00 | 43.21 | 7 |
| | ATOM | 1543 | CA | VAL B 458 | -26.706 | 89.739 | 8.351 | 1.00 | 44.98 | 6 |
| | ATOM | 1544 | CB | VAL B 458 | -27.075 | 88.255 | 8.432 | 1.00 | 44.83 | 6 |
| 45 | ATOM | 1545 | CG1 | VAL B 458 | -26.440 | 87.623 | 9.646 | 1.00 | 49.72 | 6 |
| | ATOM | 1546 | CG2 | VAL B 458 | -28.562 | 88.086 | 8.474 | 1.00 | 40.89 | 6 |
| | ATOM | 1547 | C | VAL B 458 | -25.190 | 89.822 | 8.311 | 1.00 | 42.72 | 6 |
| | ATOM | 1548 | O | VAL B 458 | -24.551 | 90.179 | 9.303 | 1.00 | 42.88 | 8 |
| | ATOM | 1549 | N | PHE B 459 | -24.605 | 89.488 | 7.180 | 1.00 | 44.53 | 7 |
| 50 | ATOM | 1550 | CA | PHE B 459 | -23.165 | 89.480 | 7.077 | 1.00 | 48.18 | 6 |
| | ATOM | 1551 | CB | PHE B 459 | -22.747 | 88.457 | 6.065 | 1.00 | 43.60 | 6 |
| | ATOM | 1552 | CG | PHE B 459 | -23.167 | 87.116 | 6.441 | 1.00 | 40.79 | 6 |
| | ATOM | 1553 | CD1 | PHE B 459 | -24.494 | 86.750 | 6.368 | 1.00 | 41.01 | 6 |
| | ATOM | 1554 | CD2 | PHE B 459 | -22.263 | 86.286 | 7.009 | 1.00 | 39.48 | 6 |
| 55 | ATOM | 1555 | CE1 | PHE B 459 | -24.892 | 85.540 | 6.889 | 1.00 | 40.62 | 6 |
| | ATOM | 1556 | CE2 | PHE B 459 | -22.649 | 85.091 | 7.527 | 1.00 | 36.87 | 6 |
| | ATOM | 1557 | CZ | PHE B 459 | -23.967 | 84.711 | 7.455 | 1.00 | 36.39 | 6 |
| | ATOM | 1558 | C | PHE B 459 | -22.627 | 90.758 | 6.623 | 1.00 | 52.71 | 6 |

| | | | | | | | | | | | | |
|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 1559 | O | PHE | B | 459 | -21.414 | 91.050 | 6.791 | 1.00 | 51.34 | 8 |
| | ATOM | 1560 | N | GLU | B | 460 | -23.489 | 91.531 | 5.976 | 1.00 | 62.92 | 7 |
| | ATOM | 1561 | CA | GLU | B | 460 | -22.953 | 92.741 | 5.533 | 1.00 | 69.33 | 6 |
| | ATOM | 1562 | CB | GLU | B | 460 | -23.851 | 93.487 | 4.505 | 1.00 | 72.95 | 6 |
| | ATOM | 1563 | CG | GLU | B | 460 | -22.917 | 94.002 | 3.412 | 1.00 | 78.35 | 6 |
| 10 | ATOM | 1564 | CD | GLU | B | 460 | -22.908 | 95.480 | 3.256 | 1.00 | 82.97 | 6 |
| | ATOM | 1565 | OE1 | GLU | B | 460 | -23.257 | 96.213 | 4.217 | 1.00 | 88.28 | 8 |
| | ATOM | 1566 | OE2 | GLU | B | 460 | -22.524 | 95.977 | 2.167 | 1.00 | 84.80 | 8 |
| | ATOM | 1567 | C | GLU | B | 460 | -22.790 | 93.576 | 6.786 | 1.00 | 71.87 | 6 |
| | ATOM | 1568 | O | GLU | B | 460 | -23.471 | 93.391 | 7.802 | 1.00 | 74.51 | 8 |
| 15 | ATOM | 1569 | N | ASP | B | 461 | -21.796 | 94.449 | 6.696 | 1.00 | 78.50 | 7 |
| | ATOM | 1570 | CA | ASP | B | 461 | -21.401 | 95.328 | 7.701 | 1.00 | 84.19 | 6 |
| | ATOM | 1571 | CB | ASP | B | 461 | -20.182 | 96.032 | 7.125 | 1.00 | 85.82 | 6 |
| | ATOM | 1572 | CG | ASP | B | 461 | -19.261 | 95.066 | 6.463 | 1.00 | 89.62 | 6 |
| | ATOM | 1573 | OD1 | ASP | B | 461 | -19.670 | 93.929 | 5.982 | 1.00 | 93.00 | 8 |
| 20 | ATOM | 1574 | OD2 | ASP | B | 461 | -18.084 | 95.361 | 6.387 | 1.00 | 93.04 | 8 |
| | ATOM | 1575 | C | ASP | B | 461 | -22.540 | 96.291 | 8.012 | 1.00 | 86.80 | 6 |
| | ATOM | 1576 | O | ASP | B | 461 | -23.063 | 96.176 | 9.139 | 1.00 | 88.70 | 8 |
| | ATOM | 1577 | OXT | ASP | B | 461 | -22.962 | 97.048 | 7.098 | 1.00 | 88.70 | 8 |
| | TER | | | | | | | | | | | |
| 25 | ATOM | 4002 | C1 | T3 | J | 1 | 20.152 | 36.643 | 29.561 | 1.00 | 22.34 | 6 |
| | ATOM | 4003 | C2 | T3 | J | 1 | 19.021 | 41.567 | 29.283 | 1.00 | 21.84 | 6 |
| | ATOM | 4004 | C3 | T3 | J | 1 | 18.880 | 37.086 | 29.226 | 1.00 | 23.43 | 6 |
| | ATOM | 4005 | C4 | T3 | J | 1 | 18.249 | 42.606 | 28.776 | 1.00 | 22.31 | 6 |
| | ATOM | 4006 | C5 | T3 | J | 1 | 18.747 | 38.372 | 28.866 | 1.00 | 24.83 | 6 |
| 30 | ATOM | 4007 | C6 | T3 | J | 1 | 17.938 | 43.621 | 29.664 | 1.00 | 25.16 | 6 |
| | ATOM | 4008 | C7 | T3 | J | 1 | 19.799 | 39.296 | 28.753 | 1.00 | 24.65 | 6 |
| | ATOM | 4009 | C8 | T3 | J | 1 | 18.330 | 43.594 | 31.028 | 1.00 | 21.93 | 6 |
| | ATOM | 4010 | C9 | T3 | J | 1 | 21.101 | 38.940 | 29.075 | 1.00 | 25.09 | 6 |
| | ATOM | 4011 | C10 | T3 | J | 1 | 19.063 | 42.558 | 31.465 | 1.00 | 23.66 | 6 |
| 35 | ATOM | 4012 | C11 | T3 | J | 1 | 21.254 | 37.600 | 29.456 | 1.00 | 23.12 | 6 |
| | ATOM | 4013 | C12 | T3 | J | 1 | 19.459 | 41.490 | 30.621 | 1.00 | 19.67 | 6 |
| | ATOM | 4014 | C13 | T3 | J | 1 | 20.370 | 35.228 | 30.075 | 1.00 | 18.97 | 6 |
| | ATOM | 4015 | C15 | T3 | J | 1 | 21.549 | 34.480 | 29.455 | 1.00 | 19.32 | 6 |
| | ATOM | 4016 | C17 | T3 | J | 1 | 21.535 | 33.003 | 29.710 | 1.00 | 19.02 | 6 |
| 40 | ATOM | 4017 | I1 | T3 | J | 1 | 16.898 | 39.029 | 28.661 | 1.00 | 25.29 | 53 |
| | ATOM | 4018 | I2 | T3 | J | 1 | 17.058 | 45.327 | 29.154 | 1.00 | 26.49 | 53 |
| | ATOM | 4019 | I3 | T3 | J | 1 | 22.763 | 40.262 | 29.169 | 1.00 | 25.67 | 53 |
| | ATOM | 4020 | N1 | T3 | J | 1 | 21.800 | 34.859 | 28.024 | 1.00 | 15.12 | 7 |
| | ATOM | 4021 | O1 | T3 | J | 1 | 17.934 | 44.682 | 31.806 | 1.00 | 21.79 | 8 |
| 45 | ATOM | 4022 | O2 | T3 | J | 1 | 19.432 | 40.560 | 28.362 | 1.00 | 22.05 | 8 |
| | ATOM | 4023 | O3 | T3 | J | 1 | 21.911 | 32.260 | 28.776 | 1.00 | 20.38 | 8 |
| | ATOM | 4024 | O4 | T3 | J | 1 | 21.137 | 32.622 | 30.840 | 1.00 | 20.16 | 8 |
| | TER | | | | | | | | | | | |
| | ATOM | 4025 | C1 | T3 | K | 1 | -28.131 | 75.928 | 7.543 | 1.00 | 22.34 | 6 |
| 50 | ATOM | 4026 | C2 | T3 | K | 1 | -24.676 | 77.673 | 4.318 | 1.00 | 21.84 | 6 |
| | ATOM | 4027 | C3 | T3 | K | 1 | -28.490 | 76.351 | 6.201 | 1.00 | 23.43 | 6 |
| | ATOM | 4028 | C4 | T3 | K | 1 | -24.217 | 77.893 | 2.989 | 1.00 | 22.31 | 6 |
| | ATOM | 4029 | C5 | T3 | K | 1 | -27.485 | 76.499 | 5.233 | 1.00 | 24.83 | 6 |
| | ATOM | 4030 | C6 | T3 | K | 1 | -23.545 | 79.124 | 2.700 | 1.00 | 25.16 | 6 |
| 55 | ATOM | 4031 | C7 | T3 | K | 1 | -26.132 | 76.227 | 5.581 | 1.00 | 24.65 | 6 |
| | ATOM | 4032 | C8 | T3 | K | 1 | -23.382 | 80.104 | 3.772 | 1.00 | 21.93 | 6 |
| | ATOM | 4033 | C9 | T3 | K | 1 | -25.685 | 75.833 | 6.855 | 1.00 | 25.09 | 6 |
| | ATOM | 4034 | C10 | T3 | K | 1 | -23.867 | 79.823 | 5.042 | 1.00 | 23.66 | 6 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|----|
| 5 | ATOM | 4035 | C11 | T3 | K | 1 | -26.708 | 75.670 | 7.834 | 1.00 | 23.12 | 6 |
| | ATOM | 4036 | C12 | T3 | K | 1 | -24.521 | 78.610 | 5.376 | 1.00 | 19.67 | 6 |
| | ATOM | 4037 | C13 | T3 | K | 1 | -29.211 | 75.830 | 8.626 | 1.00 | 18.97 | 6 |
| | ATOM | 4038 | C15 | T3 | K | 1 | -29.181 | 74.567 | 9.488 | 1.00 | 19.32 | 6 |
| | ATOM | 4039 | C17 | T3 | K | 1 | -30.440 | 74.343 | 10.264 | 1.00 | 19.02 | 6 |
| 10 | ATOM | 4040 | I1 | T3 | K | 1 | -27.868 | 77.342 | 3.316 | 1.00 | 25.29 | 53 |
| | ATOM | 4041 | I2 | T3 | K | 1 | -22.732 | 79.619 | 0.850 | 1.00 | 26.49 | 53 |
| | ATOM | 4042 | I3 | T3 | K | 1 | -23.602 | 75.792 | 7.334 | 1.00 | 25.67 | 53 |
| | ATOM | 4043 | N1 | T3 | K | 1 | -28.680 | 73.342 | 8.762 | 1.00 | 15.12 | 7 |
| | ATOM | 4044 | O1 | T3 | K | 1 | -22.742 | 81.265 | 3.443 | 1.00 | 21.79 | 8 |
| 15 | ATOM | 4045 | O2 | T3 | K | 1 | -25.267 | 76.388 | 4.595 | 1.00 | 22.05 | 8 |
| | ATOM | 4046 | O3 | T3 | K | 1 | -30.816 | 73.159 | 10.382 | 1.00 | 20.38 | 8 |
| | ATOM | 4047 | O4 | T3 | K | 1 | -31.028 | 75.359 | 10.729 | 1.00 | 20.16 | 8 |
| | TER | | | | | | | | | | | |
| | ATOM | 1 | C | LYS | X | 686 | 13.868 | 40.176 | 48.888 | 1.00 | 40.00 | 6 |
| 20 | ATOM | 2 | O | LYS | X | 686 | 13.914 | 40.120 | 47.639 | 1.00 | 40.00 | 8 |
| | ATOM | 3 | N | LYS | X | 686 | 14.374 | 42.245 | 50.489 | 1.00 | 40.00 | 7 |
| | ATOM | 4 | CA | LYS | X | 686 | 14.937 | 41.070 | 49.710 | 1.00 | 40.00 | 6 |
| | ATOM | 5 | N | HIS | X | 687 | 13.038 | 39.527 | 49.705 | 1.00 | 40.00 | 7 |
| | ATOM | 6 | CA | HIS | X | 687 | 11.891 | 38.518 | 49.521 | 1.00 | 40.00 | 6 |
| 25 | ATOM | 7 | CB | HIS | X | 687 | 10.639 | 39.000 | 50.212 | 1.00 | 40.00 | 6 |
| | ATOM | 8 | CG | HIS | X | 687 | 10.981 | 39.526 | 51.563 | 1.00 | 40.00 | 6 |
| | ATOM | 9 | CD2 | HIS | X | 687 | 11.021 | 38.908 | 52.753 | 1.00 | 40.00 | 6 |
| | ATOM | 10 | ND1 | HIS | X | 687 | 11.354 | 40.844 | 51.754 | 1.00 | 40.00 | 7 |
| | ATOM | 11 | CE1 | HIS | X | 687 | 11.614 | 40.994 | 53.034 | 1.00 | 40.00 | 6 |
| 30 | ATOM | 12 | NE2 | HIS | X | 687 | 11.422 | 39.847 | 53.646 | 1.00 | 40.00 | 7 |
| | ATOM | 13 | C | HIS | X | 687 | 11.183 | 38.108 | 48.208 | 1.00 | 40.00 | 6 |
| | ATOM | 14 | O | HIS | X | 687 | 11.674 | 38.361 | 47.094 | 1.00 | 40.00 | 8 |
| | ATOM | 15 | N | LYS | X | 688 | 10.064 | 37.458 | 48.649 | 1.00 | 40.00 | 7 |
| | ATOM | 16 | CA | LYS | X | 688 | 8.911 | 36.858 | 47.931 | 1.00 | 40.00 | 6 |
| 35 | ATOM | 17 | CB | LYS | X | 688 | 8.292 | 37.850 | 46.968 | 1.00 | 40.00 | 6 |
| | ATOM | 18 | C | LYS | X | 688 | 9.246 | 35.573 | 47.161 | 1.00 | 40.00 | 6 |
| | ATOM | 19 | O | LYS | X | 688 | 9.319 | 34.473 | 47.722 | 1.00 | 40.00 | 8 |
| | ATOM | 20 | N | ILE | X | 689 | 9.426 | 35.754 | 45.865 | 1.00 | 40.00 | 7 |
| | ATOM | 21 | CA | ILE | X | 689 | 9.661 | 34.640 | 44.924 | 1.00 | 40.00 | 6 |
| 40 | ATOM | 22 | CB | ILE | X | 689 | 9.731 | 35.167 | 43.498 | 1.00 | 40.00 | 6 |
| | ATOM | 23 | CG2 | ILE | X | 689 | 9.638 | 34.053 | 42.453 | 1.00 | 40.00 | 6 |
| | ATOM | 24 | CG1 | ILE | X | 689 | 8.597 | 36.141 | 43.176 | 1.00 | 40.00 | 6 |
| | ATOM | 25 | CD1 | ILE | X | 689 | 8.250 | 36.183 | 41.688 | 1.00 | 40.00 | 6 |
| | ATOM | 26 | C | ILE | X | 689 | 10.954 | 33.869 | 45.228 | 1.00 | 40.00 | 6 |
| 45 | ATOM | 27 | O | ILE | X | 689 | 10.920 | 32.657 | 45.511 | 1.00 | 40.00 | 8 |
| | ATOM | 28 | N | LEU | X | 690 | 12.065 | 34.579 | 45.140 | 1.00 | 40.00 | 7 |
| | ATOM | 29 | CA | LEU | X | 690 | 13.391 | 33.996 | 45.397 | 1.00 | 40.00 | 6 |
| | ATOM | 30 | CB | LEU | X | 690 | 14.349 | 35.043 | 45.892 | 1.00 | 40.00 | 6 |
| | ATOM | 31 | CG | LEU | X | 690 | 14.450 | 36.168 | 44.906 | 1.00 | 40.00 | 6 |
| 50 | ATOM | 32 | CD1 | LEU | X | 690 | 15.397 | 37.261 | 45.363 | 1.00 | 40.00 | 6 |
| | ATOM | 33 | CD2 | LEU | X | 690 | 14.940 | 35.695 | 43.540 | 1.00 | 40.00 | 6 |
| | ATOM | 34 | C | LEU | X | 690 | 13.271 | 32.999 | 46.466 | 1.00 | 40.00 | 6 |
| | ATOM | 35 | O | LEU | X | 690 | 13.633 | 31.832 | 46.315 | 1.00 | 40.00 | 8 |
| | ATOM | 36 | N | HIS | X | 691 | 12.773 | 33.472 | 47.541 | 1.00 | 40.00 | 7 |
| 55 | ATOM | 37 | CA | HIS | X | 691 | 12.557 | 32.559 | 48.569 | 1.00 | 40.00 | 6 |
| | ATOM | 38 | CB | HIS | X | 691 | 11.729 | 33.212 | 49.658 | 1.00 | 40.00 | 6 |
| | ATOM | 39 | CG | HIS | X | 691 | 12.588 | 34.116 | 50.564 | 1.00 | 40.00 | 6 |
| | ATOM | 40 | CD2 | HIS | X | 691 | 13.648 | 33.852 | 51.385 | 1.00 | 40.00 | 6 |

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|----|------|----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 41 | ND1 | HIS | X | 691 | 12.359 | 35.484 | 50.669 | 1.00 | 40.00 | 7 |
| | ATOM | 42 | CE1 | HIS | X | 691 | 13.242 | 35.991 | 51.513 | 1.00 | 40.00 | 6 |
| | ATOM | 43 | NE2 | HIS | X | 691 | 14.016 | 35.031 | 51.949 | 1.00 | 40.00 | 7 |
| | ATOM | 44 | C | HIS | X | 691 | 11.954 | 31.331 | 47.861 | 1.00 | 40.00 | 6 |
| | ATOM | 45 | O | HIS | X | 691 | 12.505 | 30.240 | 47.882 | 1.00 | 40.00 | 8 |
| 10 | ATOM | 46 | N | ARG | X | 692 | 10.839 | 31.494 | 47.167 | 1.00 | 40.00 | 7 |
| | ATOM | 47 | CA | ARG | X | 692 | 10.169 | 30.333 | 46.518 | 1.00 | 40.00 | 6 |
| | ATOM | 48 | CB | ARG | X | 692 | 9.118 | 30.800 | 45.517 | 1.00 | 40.00 | 6 |
| | ATOM | 49 | C | ARG | X | 692 | 11.153 | 29.402 | 45.752 | 1.00 | 40.00 | 6 |
| | ATOM | 50 | O | ARG | X | 692 | 11.030 | 28.168 | 45.779 | 1.00 | 40.00 | 8 |
| 15 | ATOM | 51 | N | LEU | X | 693 | 12.117 | 30.000 | 45.072 | 1.00 | 40.00 | 7 |
| | ATOM | 52 | CA | LEU | X | 693 | 13.078 | 29.252 | 44.226 | 1.00 | 40.00 | 6 |
| | ATOM | 53 | CB | LEU | X | 693 | 13.784 | 30.210 | 43.274 | 1.00 | 40.00 | 6 |
| | ATOM | 54 | CG | LEU | X | 693 | 12.796 | 31.012 | 42.432 | 1.00 | 40.00 | 6 |
| | ATOM | 55 | CD1 | LEU | X | 693 | 13.479 | 31.969 | 41.458 | 1.00 | 40.00 | 6 |
| 20 | ATOM | 56 | CD2 | LEU | X | 693 | 11.884 | 30.126 | 41.579 | 1.00 | 40.00 | 6 |
| | ATOM | 57 | C | LEU | X | 693 | 14.143 | 28.531 | 45.054 | 1.00 | 40.00 | 6 |
| | ATOM | 58 | O | LEU | X | 693 | 14.702 | 27.508 | 44.633 | 1.00 | 40.00 | 8 |
| | ATOM | 59 | N | LEU | X | 694 | 14.400 | 29.079 | 46.209 | 1.00 | 40.00 | 7 |
| | ATOM | 60 | CA | LEU | X | 694 | 15.407 | 28.538 | 47.115 | 1.00 | 40.00 | 6 |
| 25 | ATOM | 61 | CB | LEU | X | 694 | 15.871 | 29.626 | 48.084 | 1.00 | 40.00 | 6 |
| | ATOM | 62 | CG | LEU | X | 694 | 16.692 | 30.716 | 47.404 | 1.00 | 40.00 | 6 |
| | ATOM | 63 | CD1 | LEU | X | 694 | 17.279 | 31.724 | 48.391 | 1.00 | 40.00 | 6 |
| | ATOM | 64 | CD2 | LEU | X | 694 | 17.879 | 30.156 | 46.619 | 1.00 | 40.00 | 6 |
| | ATOM | 65 | C | LEU | X | 694 | 14.837 | 27.404 | 47.957 | 1.00 | 40.00 | 6 |
| 30 | ATOM | 66 | O | LEU | X | 694 | 15.555 | 26.747 | 48.716 | 1.00 | 40.00 | 8 |
| | ATOM | 67 | N | GLN | X | 695 | 13.554 | 27.157 | 47.809 | 1.00 | 40.00 | 7 |
| | ATOM | 68 | CA | GLN | X | 695 | 12.883 | 26.188 | 48.685 | 1.00 | 40.00 | 6 |
| | ATOM | 69 | C | GLN | X | 695 | 12.423 | 24.910 | 47.977 | 1.00 | 40.00 | 6 |
| | ATOM | 70 | O | GLN | X | 695 | 12.309 | 23.845 | 48.598 | 1.00 | 40.00 | 8 |
| 35 | ATOM | 71 | CB | GLN | X | 695 | 11.681 | 26.858 | 49.322 | 1.00 | 40.00 | 6 |
| | ATOM | 72 | CG | GLN | X | 695 | 12.074 | 28.125 | 50.080 | 1.00 | 20.00 | 6 |
| | ATOM | 73 | CD | GLN | X | 695 | 10.899 | 28.768 | 50.801 | 1.00 | 20.00 | 6 |
| | ATOM | 74 | OE1 | GLN | X | 695 | 9.772 | 28.296 | 50.671 | 1.00 | 20.00 | 8 |
| | ATOM | 75 | NE2 | GLN | X | 695 | 11.092 | 29.828 | 51.560 | 1.00 | 20.00 | 7 |
| 40 | ATOM | 76 | N | ASP | X | 696 | 12.155 | 25.020 | 46.714 | 1.00 | 40.00 | 7 |
| | ATOM | 77 | CA | ASP | X | 696 | 11.698 | 23.885 | 45.910 | 1.00 | 40.00 | 6 |
| | ATOM | 78 | CB | ASP | X | 696 | 11.450 | 24.400 | 44.497 | 1.00 | 40.00 | 6 |
| | ATOM | 79 | CG | ASP | X | 696 | 10.782 | 23.411 | 43.548 | 1.00 | 40.00 | 6 |
| | ATOM | 80 | OD1 | ASP | X | 696 | 10.550 | 22.203 | 43.920 | 1.00 | 40.00 | 8 |
| 45 | ATOM | 81 | OD2 | ASP | X | 696 | 10.449 | 23.804 | 42.362 | 1.00 | 40.00 | 8 |
| | ATOM | 82 | C | ASP | X | 696 | 12.774 | 22.806 | 45.876 | 1.00 | 40.00 | 6 |
| | ATOM | 83 | O | ASP | X | 696 | 13.937 | 23.077 | 45.562 | 1.00 | 40.00 | 8 |
| | ATOM | 84 | N | SER | X | 697 | 12.370 | 21.610 | 46.213 | 1.00 | 40.00 | 7 |
| | ATOM | 85 | CA | SER | X | 697 | 13.258 | 20.453 | 46.128 | 1.00 | 40.00 | 6 |
| 50 | ATOM | 86 | CB | SER | X | 697 | 12.685 | 19.371 | 47.049 | 1.00 | 40.00 | 6 |
| | ATOM | 87 | OG | SER | X | 697 | 12.535 | 19.899 | 48.374 | 1.00 | 40.00 | 8 |
| | ATOM | 88 | C | SER | X | 697 | 13.329 | 20.130 | 44.613 | 1.00 | 40.00 | 6 |
| | ATOM | 89 | O | SER | X | 697 | 14.247 | 20.573 | 43.914 | 1.00 | 40.00 | 8 |
| | ATOM | 90 | N | SER | X | 698 | 12.355 | 19.357 | 44.183 | 1.00 | 40.00 | 7 |
| 55 | ATOM | 91 | CA | SER | X | 698 | 11.985 | 19.100 | 42.752 | 1.00 | 40.00 | 6 |
| | ATOM | 92 | CB | SER | X | 698 | 11.693 | 20.417 | 42.036 | 1.00 | 40.00 | 6 |
| | ATOM | 93 | OG | SER | X | 698 | 10.510 | 21.000 | 42.577 | 1.00 | 40.00 | 8 |
| | ATOM | 94 | C | SER | X | 698 | 12.887 | 18.340 | 41.758 | 1.00 | 40.00 | 6 |

| | | | | | | | | | | | | |
|----|------|----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 95 | O | SER | X | 698 | 13.253 | 17.158 | 42.026 | 1.00 | 40.00 | 8 |
| | ATOM | 96 | OXT | SER | X | 698 | 13.131 | 18.976 | 40.714 | 1.00 | 40.00 | 8 |
| | TER | | | | | | | | | | | |
| | ATOM | 1 | CB | LYS | Y | 688 | -33.793 | 96.885 | 6.491 | 1.00 | 40.00 | 6 |
| | ATOM | 2 | C | LYS | Y | 688 | -35.002 | 95.370 | 8.130 | 1.00 | 40.00 | 6 |
| 10 | ATOM | 3 | O | LYS | Y | 688 | -36.027 | 95.520 | 8.779 | 1.00 | 40.00 | 8 |
| | ATOM | 4 | N | LYS | Y | 688 | -32.717 | 96.619 | 8.695 | 1.00 | 40.00 | 7 |
| | ATOM | 5 | CA | LYS | Y | 688 | -34.040 | 96.591 | 7.954 | 1.00 | 40.00 | 6 |
| | ATOM | 6 | N | ILE | Y | 689 | -34.578 | 93.781 | 6.908 | 1.00 | 40.00 | 7 |
| | ATOM | 7 | CA | ILE | Y | 689 | -35.862 | 93.106 | 7.268 | 1.00 | 40.00 | 6 |
| 15 | ATOM | 8 | CB | ILE | Y | 689 | -35.971 | 91.759 | 6.572 | 1.00 | 40.00 | 6 |
| | ATOM | 9 | CG2 | ILE | Y | 689 | -37.270 | 91.077 | 6.932 | 1.00 | 40.00 | 6 |
| | ATOM | 10 | CG1 | ILE | Y | 689 | -35.917 | 91.937 | 5.062 | 1.00 | 40.00 | 6 |
| | ATOM | 11 | CD1 | ILE | Y | 689 | -36.341 | 90.691 | 4.289 | 1.00 | 40.00 | 6 |
| | ATOM | 12 | C | ILE | Y | 689 | -36.032 | 92.870 | 8.780 | 1.00 | 40.00 | 6 |
| 20 | ATOM | 13 | O | ILE | Y | 689 | -36.913 | 93.446 | 9.442 | 1.00 | 40.00 | 8 |
| | ATOM | 14 | N | LEU | Y | 690 | -35.019 | 92.834 | 9.787 | 1.00 | 40.00 | 7 |
| | ATOM | 15 | CA | LEU | Y | 690 | -34.956 | 92.320 | 11.163 | 1.00 | 40.00 | 6 |
| | ATOM | 16 | CB | LEU | Y | 690 | -33.528 | 92.432 | 11.697 | 1.00 | 40.00 | 6 |
| | ATOM | 17 | CG | LEU | Y | 690 | -32.516 | 91.647 | 10.864 | 1.00 | 40.00 | 6 |
| 25 | ATOM | 18 | CD1 | LEU | Y | 690 | -31.087 | 91.764 | 11.397 | 1.00 | 40.00 | 6 |
| | ATOM | 19 | CD2 | LEU | Y | 690 | -32.819 | 90.148 | 10.812 | 1.00 | 40.00 | 6 |
| | ATOM | 20 | C | LEU | Y | 690 | -35.899 | 93.123 | 12.065 | 1.00 | 40.00 | 6 |
| | ATOM | 21 | O | LEU | Y | 690 | -36.570 | 92.492 | 12.928 | 1.00 | 40.00 | 8 |
| | ATOM | 22 | N | HIS | Y | 691 | -36.039 | 94.731 | 11.373 | 1.00 | 40.00 | 7 |
| 30 | ATOM | 23 | CA | HIS | Y | 691 | -36.634 | 94.923 | 12.683 | 1.00 | 40.00 | 6 |
| | ATOM | 24 | CB | HIS | Y | 691 | -36.854 | 96.383 | 12.935 | 1.00 | 40.00 | 6 |
| | ATOM | 25 | CG | HIS | Y | 691 | -35.610 | 97.153 | 13.078 | 1.00 | 40.00 | 6 |
| | ATOM | 26 | CD2 | HIS | Y | 691 | -34.757 | 97.640 | 12.159 | 1.00 | 40.00 | 6 |
| | ATOM | 27 | ND1 | HIS | Y | 691 | -35.129 | 97.579 | 14.319 | 1.00 | 40.00 | 7 |
| 35 | ATOM | 28 | CE1 | HIS | Y | 691 | -34.039 | 98.290 | 14.122 | 1.00 | 40.00 | 6 |
| | ATOM | 29 | NE2 | HIS | Y | 691 | -33.786 | 98.346 | 12.815 | 1.00 | 40.00 | 7 |
| | ATOM | 30 | C | HIS | Y | 691 | -37.972 | 94.287 | 12.756 | 1.00 | 40.00 | 6 |
| | ATOM | 31 | O | HIS | Y | 691 | -38.240 | 93.417 | 13.545 | 1.00 | 40.00 | 8 |
| | ATOM | 32 | N | ARG | Y | 692 | -38.265 | 94.388 | 11.505 | 1.00 | 40.00 | 7 |
| 40 | ATOM | 33 | CA | ARG | Y | 692 | -39.577 | 93.869 | 11.276 | 1.00 | 40.00 | 6 |
| | ATOM | 34 | CB | ARG | Y | 692 | -39.653 | 93.692 | 9.795 | 1.00 | 40.00 | 6 |
| | ATOM | 35 | CG | ARG | Y | 692 | -40.759 | 92.764 | 9.329 | 1.00 | 40.00 | 6 |
| | ATOM | 36 | CD | ARG | Y | 692 | -40.618 | 92.422 | 7.848 | 1.00 | 40.00 | 6 |
| | ATOM | 37 | NE | ARG | Y | 692 | -41.849 | 92.641 | 7.091 | 1.00 | 40.00 | 7 |
| 45 | ATOM | 38 | CZ | ARG | Y | 692 | -41.898 | 92.758 | 5.763 | 1.00 | 40.00 | 6 |
| | ATOM | 39 | NH1 | ARG | Y | 692 | -40.784 | 92.695 | 5.024 | 1.00 | 40.00 | 7 |
| | ATOM | 40 | NH2 | ARG | Y | 692 | -43.034 | 92.940 | 5.080 | 1.00 | 40.00 | 7 |
| | ATOM | 41 | C | ARG | Y | 692 | -39.941 | 92.547 | 11.995 | 1.00 | 40.00 | 6 |
| | ATOM | 42 | O | ARG | Y | 692 | -41.001 | 92.440 | 12.649 | 1.00 | 40.00 | 8 |
| 50 | ATOM | 43 | N | LEU | Y | 693 | -39.095 | 91.576 | 11.816 | 1.00 | 40.00 | 7 |
| | ATOM | 44 | CA | LEU | Y | 693 | -39.230 | 90.232 | 12.395 | 1.00 | 40.00 | 6 |
| | ATOM | 45 | CB | LEU | Y | 693 | -38.362 | 89.337 | 11.615 | 1.00 | 40.00 | 6 |
| | ATOM | 46 | CG | LEU | Y | 693 | -38.737 | 89.375 | 10.132 | 1.00 | 40.00 | 6 |
| | ATOM | 47 | CD1 | LEU | Y | 693 | -37.794 | 88.570 | 9.247 | 1.00 | 40.00 | 6 |
| 55 | ATOM | 48 | CD2 | LEU | Y | 693 | -40.142 | 88.827 | 9.862 | 1.00 | 40.00 | 6 |
| | ATOM | 49 | C | LEU | Y | 693 | -38.921 | 90.378 | 13.816 | 1.00 | 40.00 | 6 |
| | ATOM | 50 | O | LEU | Y | 693 | -39.191 | 89.474 | 14.615 | 1.00 | 40.00 | 8 |
| | ATOM | 51 | N | LEU | Y | 694 | -38.366 | 91.533 | 14.076 | 1.00 | 40.00 | 7 |

| | | | | | | | | | | | | |
|----|------|----|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| 5 | ATOM | 52 | CA | LEU | Y | 694 | -38.174 | 91.885 | 15.435 | 1.00 | 40.00 | 6 |
| | ATOM | 53 | CB | LEU | Y | 694 | -37.181 | 93.002 | 15.561 | 1.00 | 40.00 | 6 |
| | ATOM | 54 | CG | LEU | Y | 694 | -35.799 | 92.377 | 15.869 | 1.00 | 40.00 | 6 |
| | ATOM | 55 | CD1 | LEU | Y | 694 | -34.897 | 93.275 | 16.702 | 1.00 | 40.00 | 6 |
| | ATOM | 56 | CD2 | LEU | Y | 694 | -35.897 | 91.055 | 16.661 | 1.00 | 40.00 | 6 |
| 10 | ATOM | 57 | C | LEU | Y | 694 | -39.596 | 91.903 | 15.915 | 1.00 | 40.00 | 6 |
| | ATOM | 58 | O | LEU | Y | 694 | -39.985 | 91.253 | 16.858 | 1.00 | 40.00 | 8 |
| | ATOM | 59 | N | GLN | Y | 695 | -40.787 | 92.229 | 15.048 | 1.00 | 40.00 | 7 |
| | ATOM | 60 | CA | GLN | Y | 695 | -42.034 | 91.457 | 15.543 | 1.00 | 40.00 | 6 |
| | ATOM | 61 | C | GLN | Y | 695 | -43.054 | 90.901 | 14.240 | 1.00 | 40.00 | 6 |
| 15 | ATOM | 62 | O | GLN | Y | 695 | -43.102 | 91.557 | 13.189 | 1.00 | 40.00 | 8 |
| | ATOM | 63 | CB | GLN | Y | 695 | -42.362 | 92.025 | 16.923 | 1.00 | 40.00 | 6 |
| | ATOM | 64 | CG | GLN | Y | 695 | -41.013 | 92.101 | 17.768 | 1.00 | 40.00 | 6 |
| | ATOM | 65 | CD | GLN | Y | 695 | -40.943 | 91.235 | 19.059 | 1.00 | 40.00 | 6 |
| | ATOM | 66 | OE1 | GLN | Y | 695 | -41.828 | 90.426 | 19.318 | 1.00 | 40.00 | 8 |
| 20 | ATOM | 67 | NE2 | GLN | Y | 695 | -39.938 | 91.399 | 19.916 | 1.00 | 40.00 | 7 |
| | ATOM | 68 | N | ASP | Y | 696 | -43.802 | 89.498 | 14.402 | 1.00 | 40.00 | 7 |
| | ATOM | 69 | CA | ASP | Y | 696 | -44.784 | 88.354 | 13.428 | 1.00 | 40.00 | 6 |
| | ATOM | 70 | C | ASP | Y | 696 | -46.034 | 88.934 | 12.759 | 1.00 | 40.00 | 6 |
| | ATOM | 71 | O | ASP | Y | 696 | -46.266 | 88.655 | 11.529 | 1.00 | 40.00 | 8 |
| 25 | ATOM | 72 | CB | ASP | Y | 696 | -45.211 | 87.192 | 14.322 | 1.00 | 40.00 | 6 |
| | ATOM | 73 | CG | ASP | Y | 696 | -44.021 | 86.560 | 15.058 | 1.00 | 40.00 | 6 |
| | ATOM | 74 | OD1 | ASP | Y | 696 | -42.823 | 86.994 | 14.844 | 1.00 | 40.00 | 8 |
| | ATOM | 75 | OD2 | ASP | Y | 696 | -44.212 | 85.591 | 15.889 | 1.00 | 40.00 | 8 |
| | END | | | | | | | | | | | |
| 30 | | | | | | | | | | | | |

5

Appendix 2.

Atomic Coordinates for Human ER α Complexed with DES, and a GRIP1 NR-box 2 Peptide

| | | | | | | | | | | | |
|----|--------|----------|----------|----------|----------|--------|--------|---------|--------|------|-------|
| | CRYST1 | 54.094 | 82.217 | 58.041 | 90.00 | 111.33 | 90.00 | P | 21 | 2 | |
| 10 | ORIGX1 | 1.000000 | 0.000000 | 0.000000 | 0.000000 | | | | | | |
| | ORIGX2 | 0.000000 | 1.000000 | 0.000000 | 0.000000 | | | | | | |
| | ORIGX3 | 0.000000 | 0.000000 | 1.000000 | 0.000000 | | | | | | |
| | SCALE1 | 0.018486 | 0.000000 | 0.007221 | 0.000000 | | | | | | |
| 15 | SCALE2 | 0.000000 | 0.012163 | 0.000000 | 0.000000 | | | | | | |
| | SCALE3 | 0.000000 | 0.000000 | 0.018497 | 0.000000 | | | | | | |
| | ATOM | 1 | CB | SER | A | 305 | 35.230 | -14.787 | -1.163 | 1.00 | 73.26 |
| | ATOM | 2 | C | SER | A | 305 | 35.331 | -14.303 | 1.289 | 1.00 | 72.95 |
| 20 | ATOM | 3 | O | SER | A | 305 | 34.146 | -13.984 | 1.186 | 1.00 | 72.46 |
| | ATOM | 4 | N | SER | A | 305 | 36.797 | -16.033 | 0.285 | 1.00 | 74.06 |
| | ATOM | 5 | CA | SER | A | 305 | 36.138 | -14.713 | 0.061 | 1.00 | 73.59 |
| | ATOM | 6 | N | LEU | A | 306 | 35.982 | -14.313 | 2.449 | 1.00 | 72.21 |
| | ATOM | 7 | CA | LEU | A | 306 | 35.329 | -13.950 | 3.702 | 1.00 | 71.05 |
| 25 | ATOM | 8 | CB | LEU | A | 306 | 36.251 | -14.256 | 4.878 | 1.00 | 70.19 |
| | ATOM | 9 | C | LEU | A | 306 | 34.929 | -12.478 | 3.719 | 1.00 | 69.57 |
| | ATOM | 10 | O | LEU | A | 306 | 35.580 | -11.638 | 3.100 | 1.00 | 69.96 |
| | ATOM | 11 | N | ALA | A | 307 | 33.851 | -12.176 | 4.434 | 1.00 | 68.06 |
| | ATOM | 12 | CA | ALA | A | 307 | 33.358 | -10.810 | 4.541 | 1.00 | 64.88 |
| 30 | ATOM | 13 | CB | ALA | A | 307 | 31.841 | -10.795 | 4.436 | 1.00 | 65.83 |
| | ATOM | 14 | C | ALA | A | 307 | 33.792 | -10.204 | 5.866 | 1.00 | 63.36 |
| | ATOM | 15 | O | ALA | A | 307 | 33.878 | -8.984 | 6.005 | 1.00 | 62.73 |
| | ATOM | 16 | N | LEU | A | 308 | 34.064 | -11.062 | 6.842 | 1.00 | 62.52 |
| | ATOM | 17 | CA | LEU | A | 308 | 34.487 | -10.598 | 8.156 | 1.00 | 62.57 |
| 35 | ATOM | 18 | CB | LEU | A | 308 | 34.423 | -11.745 | 9.171 | 1.00 | 62.81 |
| | ATOM | 19 | CG | LEU | A | 308 | 33.214 | -12.688 | 9.130 | 1.00 | 64.21 |
| | ATOM | 20 | CD1 | LEU | A | 308 | 33.188 | -13.513 | 10.406 | 1.00 | 66.28 |
| | ATOM | 21 | CD2 | LEU | A | 308 | 31.919 | -11.898 | 8.989 | 1.00 | 63.80 |
| | ATOM | 22 | C | LEU | A | 308 | 35.903 | -10.037 | 8.100 | 1.00 | 61.61 |
| 40 | ATOM | 23 | O | LEU | A | 308 | 36.385 | -9.445 | 9.066 | 1.00 | 62.92 |
| | ATOM | 24 | N | SER | A | 309 | 36.561 | -10.219 | 6.959 | 1.00 | 60.50 |
| | ATOM | 25 | CA | SER | A | 309 | 37.928 | -9.743 | 6.771 | 1.00 | 58.73 |
| | ATOM | 26 | CB | SER | A | 309 | 38.720 | -10.750 | 5.934 | 1.00 | 59.53 |
| | ATOM | 27 | OG | SER | A | 309 | 38.889 | -10.283 | 4.606 | 1.00 | 59.47 |
| 45 | ATOM | 28 | C | SER | A | 309 | 37.986 | -8.373 | 6.099 | 1.00 | 57.05 |
| | ATOM | 29 | O | SER | A | 309 | 38.965 | -7.637 | 6.249 | 1.00 | 56.70 |
| | ATOM | 30 | N | LEU | A | 310 | 36.940 | -8.038 | 5.352 | 1.00 | 52.69 |
| | ATOM | 31 | CA | LEU | A | 310 | 36.877 | -6.759 | 4.658 | 1.00 | 48.20 |
| | ATOM | 32 | CB | LEU | A | 310 | 35.516 | -6.596 | 3.974 | 1.00 | 48.32 |
| 50 | ATOM | 33 | CG | LEU | A | 310 | 35.301 | -7.188 | 2.583 | 1.00 | 44.94 |
| | ATOM | 34 | CD1 | LEU | A | 310 | 33.951 | -6.728 | 2.055 | 1.00 | 46.45 |
| | ATOM | 35 | CD2 | LEU | A | 310 | 36.417 | -6.755 | 1.650 | 1.00 | 43.19 |
| | ATOM | 36 | C | LEU | A | 310 | 37.086 | -5.589 | 5.609 | 1.00 | 46.44 |
| | ATOM | 37 | O | LEU | A | 310 | 36.605 | -5.607 | 6.741 | 1.00 | 46.78 |
| 55 | ATOM | 38 | N | THR | A | 311 | 37.812 | -4.576 | 5.148 | 1.00 | 44.36 |
| | ATOM | 39 | CA | THR | A | 311 | 38.034 | -3.380 | 5.949 | 1.00 | 42.88 |
| | ATOM | 40 | CB | THR | A | 311 | 39.313 | -2.633 | 5.532 | 1.00 | 42.31 |
| | ATOM | 41 | OG1 | THR | A | 311 | 39.079 | -1.936 | 4.303 | 1.00 | 42.50 |
| | ATOM | 42 | CG2 | THR | A | 311 | 40.464 | -3.606 | 5.350 | 1.00 | 46.02 |
| 60 | ATOM | 43 | C | THR | A | 311 | 36.834 | -2.475 | 5.674 | 1.00 | 43.21 |

| | | | | | | | | | | | |
|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 44 | O | THR | A | 311 | 36.021 | -2.776 | 4.800 | 1.00 | 42.12 |
| | ATOM | 45 | N | ALA | A | 312 | 36.726 | -1.372 | 6.409 | 1.00 | 42.16 |
| | ATOM | 46 | CA | ALA | A | 312 | 35.616 | -0.444 | 6.228 | 1.00 | 40.10 |
| | ATOM | 47 | CB | ALA | A | 312 | 35.741 | 0.709 | 7.205 | 1.00 | 40.07 |
| | ATOM | 48 | C | ALA | A | 312 | 35.561 | 0.090 | 4.799 | 1.00 | 41.80 |
| 10 | ATOM | 49 | O | ALA | A | 312 | 34.510 | 0.074 | 4.154 | 1.00 | 37.81 |
| | ATOM | 50 | N | ASP | A | 313 | 36.698 | 0.564 | 4.304 | 1.00 | 42.35 |
| | ATOM | 51 | CA | ASP | A | 313 | 36.752 | 1.104 | 2.953 | 1.00 | 42.27 |
| | ATOM | 52 | CB | ASP | A | 313 | 38.133 | 1.703 | 2.680 | 1.00 | 43.74 |
| | ATOM | 53 | CG | ASP | A | 313 | 38.323 | 3.054 | 3.348 | 1.00 | 46.62 |
| 15 | ATOM | 54 | OD1 | ASP | A | 313 | 39.414 | 3.645 | 3.205 | 1.00 | 51.01 |
| | ATOM | 55 | OD2 | ASP | A | 313 | 37.380 | 3.529 | 4.015 | 1.00 | 48.89 |
| | ATOM | 56 | C | ASP | A | 313 | 36.422 | 0.027 | 1.926 | 1.00 | 38.68 |
| | ATOM | 57 | O | ASP | A | 313 | 35.704 | 0.281 | 0.959 | 1.00 | 38.75 |
| | ATOM | 58 | N | GLN | A | 314 | 36.931 | -1.179 | 2.145 | 1.00 | 34.76 |
| 20 | ATOM | 59 | CA | GLN | A | 314 | 36.666 | -2.277 | 1.229 | 1.00 | 33.55 |
| | ATOM | 60 | CB | GLN | A | 314 | 37.462 | -3.512 | 1.643 | 1.00 | 36.90 |
| | ATOM | 61 | CG | GLN | A | 314 | 38.963 | -3.384 | 1.436 | 1.00 | 40.45 |
| | ATOM | 62 | CD | GLN | A | 314 | 39.700 | -4.610 | 1.905 | 1.00 | 43.13 |
| | ATOM | 63 | OE1 | GLN | A | 314 | 39.394 | -5.196 | 2.935 | 1.00 | 43.60 |
| 25 | ATOM | 64 | NE2 | GLN | A | 314 | 40.701 | -5.032 | 1.117 | 1.00 | 44.03 |
| | ATOM | 65 | C | GLN | A | 314 | 35.176 | -2.595 | 1.201 | 1.00 | 34.95 |
| | ATOM | 66 | O | GLN | A | 314 | 34.605 | -2.860 | 0.140 | 1.00 | 32.89 |
| | ATOM | 67 | N | MET | A | 315 | 34.542 | -2.564 | 2.374 | 1.00 | 32.54 |
| | ATOM | 68 | CA | MET | A | 315 | 33.115 | -2.848 | 2.470 | 1.00 | 35.46 |
| 30 | ATOM | 69 | CB | MET | A | 315 | 32.650 | -2.794 | 3.926 | 1.00 | 37.09 |
| | ATOM | 70 | CG | MET | A | 315 | 31.137 | -2.777 | 4.097 | 1.00 | 39.42 |
| | ATOM | 71 | SD | MET | A | 315 | 30.443 | -4.426 | 4.053 | 1.00 | 46.55 |
| | ATOM | 72 | CE | MET | A | 315 | 31.351 | -5.205 | 5.397 | 1.00 | 45.29 |
| | ATOM | 73 | C | MET | A | 315 | 32.311 | -1.859 | 1.640 | 1.00 | 31.83 |
| 35 | ATOM | 74 | O | MET | A | 315 | 31.453 | -2.247 | 0.852 | 1.00 | 32.10 |
| | ATOM | 75 | N | VAL | A | 316 | 32.587 | -0.560 | 1.830 | 1.00 | 32.62 |
| | ATOM | 76 | CA | VAL | A | 316 | 31.882 | 0.470 | 1.079 | 1.00 | 31.09 |
| | ATOM | 77 | CB | VAL | A | 316 | 32.395 | 1.888 | 1.425 | 1.00 | 34.77 |
| | ATOM | 78 | CG1 | VAL | A | 316 | 31.786 | 2.899 | 0.461 | 1.00 | 34.10 |
| 40 | ATOM | 79 | CG2 | VAL | A | 316 | 32.021 | 2.246 | 2.862 | 1.00 | 34.40 |
| | ATOM | 80 | C | VAL | A | 316 | 32.092 | 0.232 | -0.414 | 1.00 | 33.48 |
| | ATOM | 81 | O | VAL | A | 316 | 31.145 | 0.266 | -1.200 | 1.00 | 32.49 |
| | ATOM | 82 | N | SER | A | 317 | 33.337 | -0.027 | -0.795 | 1.00 | 33.49 |
| | ATOM | 83 | CA | SER | A | 317 | 33.682 | -0.280 | -2.187 | 1.00 | 32.88 |
| 45 | ATOM | 84 | CB | SER | A | 317 | 35.165 | -0.635 | -2.297 | 1.00 | 35.77 |
| | ATOM | 85 | OG | SER | A | 317 | 35.825 | 0.277 | -3.154 | 1.00 | 42.70 |
| | ATOM | 86 | C | SER | A | 317 | 32.849 | -1.396 | -2.801 | 1.00 | 30.71 |
| | ATOM | 87 | O | SER | A | 317 | 32.279 | -1.238 | -3.880 | 1.00 | 31.14 |
| | ATOM | 88 | N | ALA | A | 318 | 32.792 | -2.529 | -2.111 | 1.00 | 29.51 |
| 50 | ATOM | 89 | CA | ALA | A | 318 | 32.035 | -3.676 | -2.580 | 1.00 | 29.93 |
| | ATOM | 90 | CB | ALA | A | 318 | 32.156 | -4.811 | -1.579 | 1.00 | 28.56 |
| | ATOM | 91 | C | ALA | A | 318 | 30.565 | -3.305 | -2.771 | 1.00 | 31.55 |
| | ATOM | 92 | O | ALA | A | 318 | 29.961 | -3.642 | -3.784 | 1.00 | 30.64 |
| | ATOM | 93 | N | LEU | A | 319 | 29.997 | -2.614 | -1.791 | 1.00 | 34.13 |
| 55 | ATOM | 94 | CA | LEU | A | 319 | 28.597 | -2.212 | -1.861 | 1.00 | 32.93 |
| | ATOM | 95 | CB | LEU | A | 319 | 28.170 | -1.576 | -0.540 | 1.00 | 31.15 |
| | ATOM | 96 | CG | LEU | A | 319 | 28.076 | -2.555 | 0.632 | 1.00 | 32.27 |
| | ATOM | 97 | CD1 | LEU | A | 319 | 27.523 | -1.840 | 1.852 | 1.00 | 32.14 |
| | ATOM | 98 | CD2 | LEU | A | 319 | 27.194 | -3.733 | 0.243 | 1.00 | 31.82 |
| 60 | ATOM | 99 | C | LEU | A | 319 | 28.340 | -1.257 | -3.020 | 1.00 | 34.41 |
| | ATOM | 100 | O | LEU | A | 319 | 27.430 | -1.475 | -3.818 | 1.00 | 35.23 |

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|----|------|-----|-----|------|---|-----|--------|--------|---------|------|-------|
| 5 | ATOM | 101 | N | LEU | A | 320 | 29.140 | -0.195 | -3.120 | 1.00 | 32.53 |
| | ATOM | 102 | CA | LEU | A | 320 | 28.972 | 0.756 | -4.212 | 1.00 | 35.33 |
| | ATOM | 103 | CB | LEU | A | 320 | 30.052 | 1.839 | -4.155 | 1.00 | 33.52 |
| | ATOM | 104 | CG | LEU | A | 320 | 29.974 | 2.899 | -3.054 | 1.00 | 34.60 |
| | ATOM | 105 | CD1 | LEU | A | 320 | 31.060 | 3.940 | -3.292 | 1.00 | 33.69 |
| 10 | ATOM | 106 | CD2 | LEU | A | 320 | 28.611 | 3.562 | -3.044 | 1.00 | 31.05 |
| | ATOM | 107 | C | LEU | A | 320 | 29.052 | 0.040 | -5.561 | 1.00 | 35.41 |
| | ATOM | 108 | O | LEU | A | 320 | 28.230 | 0.271 | -6.446 | 1.00 | 39.16 |
| | ATOM | 109 | N | AASP | A | 321 | 30.042 | -0.833 | -5.720 | 0.50 | 36.33 |
| | ATOM | 110 | N | BASP | A | 321 | 30.041 | -0.839 | -5.695 | 0.50 | 35.76 |
| 15 | ATOM | 111 | CA | AASP | A | 321 | 30.214 | -1.559 | -6.977 | 0.50 | 37.71 |
| | ATOM | 112 | CA | BASP | A | 321 | 30.258 | -1.595 | -6.925 | 0.50 | 37.11 |
| | ATOM | 113 | CB | AASP | A | 321 | 31.537 | -2.334 | -6.973 | 0.50 | 40.01 |
| | ATOM | 114 | CB | BASP | A | 321 | 31.573 | -2.374 | -6.826 | 0.50 | 39.41 |
| | ATOM | 115 | CG | AASP | A | 321 | 31.694 | -3.230 | -8.195 | 0.50 | 41.93 |
| 20 | ATOM | 116 | CG | BASP | A | 321 | 32.770 | -1.562 | -7.284 | 0.50 | 39.96 |
| | ATOM | 117 | OD1 | AASP | A | 321 | 31.523 | -2.733 | -9.329 | 0.50 | 42.11 |
| | ATOM | 118 | OD1 | BASP | A | 321 | 33.312 | -1.868 | -8.366 | 0.50 | 43.41 |
| | ATOM | 119 | OD2 | AASP | A | 321 | 31.988 | -4.432 | -8.022 | 0.50 | 42.69 |
| | ATOM | 120 | OD2 | BASP | A | 321 | 33.170 | -0.622 | -6.564 | 0.50 | 41.33 |
| 25 | ATOM | 121 | C | AASP | A | 321 | 29.069 | -2.524 | -7.275 | 0.50 | 37.19 |
| | ATOM | 122 | C | BASP | A | 321 | 29.123 | -2.565 | -7.253 | 0.50 | 36.68 |
| | ATOM | 123 | O | AASP | A | 321 | 28.820 | -2.861 | -8.434 | 0.50 | 36.87 |
| | ATOM | 124 | O | BASP | A | 321 | 28.934 | -2.942 | -8.411 | 0.50 | 36.08 |
| | ATOM | 125 | N | ALA | A | 322 | 28.374 | -2.968 | -6.235 | 1.00 | 35.35 |
| 30 | ATOM | 126 | CA | ALA | A | 322 | 27.268 | -3.902 | -6.417 | 1.00 | 31.59 |
| | ATOM | 127 | CB | ALA | A | 322 | 27.124 | -4.781 | -5.175 | 1.00 | 30.73 |
| | ATOM | 128 | C | ALA | A | 322 | 25.946 | -3.204 | -6.709 | 1.00 | 30.07 |
| | ATOM | 129 | O | ALA | A | 322 | 24.955 | -3.857 | -7.036 | 1.00 | 26.53 |
| | ATOM | 130 | N | GLU | A | 323 | 25.932 | -1.880 | -6.596 | 1.00 | 27.98 |
| 35 | ATOM | 131 | CA | GLU | A | 323 | 24.713 | -1.117 | -6.827 | 1.00 | 29.88 |
| | ATOM | 132 | CB | GLU | A | 323 | 25.027 | 0.380 | -6.855 | 1.00 | 30.98 |
| | ATOM | 133 | CG | GLU | A | 323 | 24.870 | 1.068 | -5.509 | 1.00 | 31.62 |
| | ATOM | 134 | CD | GLU | A | 323 | 23.463 | 0.940 | -4.960 | 1.00 | 31.98 |
| | ATOM | 135 | OE1 | GLU | A | 323 | 23.183 | -0.056 | -4.257 | 1.00 | 33.10 |
| 40 | ATOM | 136 | OE2 | GLU | A | 323 | 22.640 | 1.836 | -5.233 | 1.00 | 30.01 |
| | ATOM | 137 | C | GLU | A | 323 | 24.010 | -1.515 | -8.123 | 1.00 | 30.86 |
| | ATOM | 138 | O | GLU | A | 323 | 24.655 | -1.705 | -9.151 | 1.00 | 28.86 |
| | ATOM | 139 | N | PRO | A | 324 | 22.674 | -1.659 | -8.083 | 1.00 | 30.66 |
| | ATOM | 140 | CD | PRO | A | 324 | 21.774 | -1.466 | -6.935 | 1.00 | 31.01 |
| 45 | ATOM | 141 | CA | PRO | A | 324 | 21.935 | -2.032 | -9.290 | 1.00 | 30.29 |
| | ATOM | 142 | CB | PRO | A | 324 | 20.613 | -2.598 | -8.760 | 1.00 | 31.42 |
| | ATOM | 143 | CG | PRO | A | 324 | 20.626 | -2.363 | -7.258 | 1.00 | 33.66 |
| | ATOM | 144 | C | PRO | A | 324 | 21.717 | -0.785 | -10.138 | 1.00 | 27.46 |
| | ATOM | 145 | O | PRO | A | 324 | 21.893 | 0.332 | -9.668 | 1.00 | 26.19 |
| 50 | ATOM | 146 | N | PRO | A | 325 | 21.335 | -0.959 | -11.403 | 1.00 | 27.80 |
| | ATOM | 147 | CD | PRO | A | 325 | 21.082 | -2.198 | -12.161 | 1.00 | 27.35 |
| | ATOM | 148 | CA | PRO | A | 325 | 21.125 | 0.242 | -12.211 | 1.00 | 25.59 |
| | ATOM | 149 | CB | PRO | A | 325 | 21.258 | -0.266 | -13.637 | 1.00 | 24.02 |
| | ATOM | 150 | CG | PRO | A | 325 | 20.773 | -1.695 | -13.559 | 1.00 | 26.00 |
| 55 | ATOM | 151 | C | PRO | A | 325 | 19.749 | 0.830 | -11.954 | 1.00 | 23.73 |
| | ATOM | 152 | O | PRO | A | 325 | 18.873 | 0.165 | -11.402 | 1.00 | 24.83 |
| | ATOM | 153 | N | ILE | A | 326 | 19.571 | 2.081 | -12.352 | 1.00 | 22.11 |
| | ATOM | 154 | CA | ILE | A | 326 | 18.296 | 2.762 | -12.212 | 1.00 | 24.01 |
| | ATOM | 155 | CB | ILE | A | 326 | 18.502 | 4.282 | -12.133 | 1.00 | 25.97 |
| 60 | ATOM | 156 | CG2 | ILE | A | 326 | 17.168 | 4.992 | -12.286 | 1.00 | 20.75 |
| | ATOM | 157 | CG1 | ILE | A | 326 | 19.189 | 4.632 | -10.805 | 1.00 | 29.31 |

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|----|------|-----|-----|-----|---|-----|--------|---------------|------|-------|
| 5 | ATOM | 158 | CD1 | ILE | A | 326 | 19.301 | 6.120-10.525 | 1.00 | 32.91 |
| | ATOM | 159 | C | ILE | A | 326 | 17.506 | 2.408-13.471 | 1.00 | 25.72 |
| | ATOM | 160 | O | ILE | A | 326 | 17.906 | 2.758-14.581 | 1.00 | 25.55 |
| | ATOM | 161 | N | LEU | A | 327 | 16.392 | 1.703-13.301 | 1.00 | 25.57 |
| | ATOM | 162 | CA | LEU | A | 327 | 15.595 | 1.279-14.439 | 1.00 | 23.80 |
| 10 | ATOM | 163 | CB | LEU | A | 327 | 14.872 | -0.029-14.104 | 1.00 | 23.96 |
| | ATOM | 164 | CG | LEU | A | 327 | 15.778 | -1.210-13.728 | 1.00 | 19.89 |
| | ATOM | 165 | CD1 | LEU | A | 327 | 14.944 | -2.462-13.583 | 1.00 | 21.19 |
| | ATOM | 166 | CD2 | LEU | A | 327 | 16.850 | -1.415-14.805 | 1.00 | 17.53 |
| | ATOM | 167 | C | LEU | A | 327 | 14.598 | 2.317-14.935 | 1.00 | 27.16 |
| 15 | ATOM | 168 | O | LEU | A | 327 | 14.161 | 3.202-14.194 | 1.00 | 25.98 |
| | ATOM | 169 | N | TYR | A | 328 | 14.251 | 2.207-16.210 | 1.00 | 26.56 |
| | ATOM | 170 | CA | TYR | A | 328 | 13.303 | 3.123-16.814 | 1.00 | 24.45 |
| | ATOM | 171 | CB | TYR | A | 328 | 13.724 | 3.465-18.245 | 1.00 | 26.72 |
| | ATOM | 172 | CG | TYR | A | 328 | 14.587 | 4.693-18.314 | 1.00 | 27.73 |
| 20 | ATOM | 173 | CD1 | TYR | A | 328 | 14.021 | 5.949-18.518 | 1.00 | 28.56 |
| | ATOM | 174 | CE1 | TYR | A | 328 | 14.798 | 7.092-18.509 | 1.00 | 29.10 |
| | ATOM | 175 | CD2 | TYR | A | 328 | 15.962 | 4.612-18.110 | 1.00 | 26.01 |
| | ATOM | 176 | CE2 | TYR | A | 328 | 16.750 | 5.753-18.098 | 1.00 | 30.63 |
| | ATOM | 177 | CZ | TYR | A | 328 | 16.157 | 6.988-18.297 | 1.00 | 30.07 |
| 25 | ATOM | 178 | OH | TYR | A | 328 | 16.917 | 8.130-18.265 | 1.00 | 37.94 |
| | ATOM | 179 | C | TYR | A | 328 | 11.923 | 2.501-16.827 | 1.00 | 24.95 |
| | ATOM | 180 | O | TYR | A | 328 | 11.774 | 1.274-16.846 | 1.00 | 27.02 |
| | ATOM | 181 | N | SER | A | 329 | 10.912 | 3.358-16.800 | 1.00 | 25.60 |
| | ATOM | 182 | CA | SER | A | 329 | 9.533 | 2.908-16.837 | 1.00 | 29.45 |
| 30 | ATOM | 183 | CB | SER | A | 329 | 8.661 | 3.858-16.020 | 1.00 | 30.80 |
| | ATOM | 184 | OG | SER | A | 329 | 7.297 | 3.721-16.364 | 1.00 | 33.74 |
| | ATOM | 185 | C | SER | A | 329 | 9.129 | 2.947-18.313 | 1.00 | 31.30 |
| | ATOM | 186 | O | SER | A | 329 | 9.908 | 3.397-19.154 | 1.00 | 27.35 |
| | ATOM | 187 | N | GLU | A | 330 | 7.930 | 2.469-18.629 | 1.00 | 32.98 |
| 35 | ATOM | 188 | CA | GLU | A | 330 | 7.459 | 2.482-20.007 | 1.00 | 35.10 |
| | ATOM | 189 | CB | GLU | A | 330 | 6.031 | 1.968-20.074 | 1.00 | 34.67 |
| | ATOM | 190 | C | GLU | A | 330 | 7.532 | 3.924-20.505 | 1.00 | 40.06 |
| | ATOM | 191 | O | GLU | A | 330 | 7.068 | 4.841-19.826 | 1.00 | 42.65 |
| | ATOM | 192 | N | TYR | A | 331 | 8.124 | 4.126-21.681 | 1.00 | 41.16 |
| 40 | ATOM | 193 | CA | TYR | A | 331 | 8.263 | 5.470-22.234 | 1.00 | 42.66 |
| | ATOM | 194 | CB | TYR | A | 331 | 9.323 | 5.482-23.350 | 1.00 | 42.54 |
| | ATOM | 195 | CG | TYR | A | 331 | 9.202 | 4.347-24.345 | 1.00 | 38.67 |
| | ATOM | 196 | CD1 | TYR | A | 331 | 10.105 | 3.284-24.334 | 1.00 | 34.66 |
| | ATOM | 197 | CE1 | TYR | A | 331 | 9.985 | 2.228-25.233 | 1.00 | 34.89 |
| 45 | ATOM | 198 | CD2 | TYR | A | 331 | 8.174 | 4.327-25.287 | 1.00 | 37.88 |
| | ATOM | 199 | CE2 | TYR | A | 331 | 8.045 | 3.276-26.193 | 1.00 | 34.65 |
| | ATOM | 200 | CZ | TYR | A | 331 | 8.950 | 2.232-26.159 | 1.00 | 30.73 |
| | ATOM | 201 | OH | TYR | A | 331 | 8.814 | 1.191-27.042 | 1.00 | 30.97 |
| | ATOM | 202 | C | TYR | A | 331 | 6.943 | 6.043-22.754 | 1.00 | 46.24 |
| 50 | ATOM | 203 | O | TYR | A | 331 | 6.018 | 5.301-23.096 | 1.00 | 45.38 |
| | ATOM | 204 | N | ASP | A | 332 | 6.868 | 7.372-22.792 | 1.00 | 49.11 |
| | ATOM | 205 | CA | ASP | A | 332 | 5.684 | 8.092-23.262 | 1.00 | 52.40 |
| | ATOM | 206 | CB | ASP | A | 332 | 5.781 | 8.321-24.772 | 1.00 | 52.86 |
| | ATOM | 207 | C | ASP | A | 332 | 4.356 | 7.410-22.926 | 1.00 | 52.90 |
| 55 | ATOM | 208 | O | ASP | A | 332 | 3.561 | 7.116-23.818 | 1.00 | 53.94 |
| | ATOM | 209 | N | PRO | A | 333 | 4.103 | 7.144-21.632 | 1.00 | 53.63 |
| | ATOM | 210 | CD | PRO | A | 333 | 4.962 | 7.418-20.465 | 1.00 | 53.63 |
| | ATOM | 211 | CA | PRO | A | 333 | 2.840 | 6.497-21.253 | 1.00 | 53.55 |
| | ATOM | 212 | CB | PRO | A | 333 | 3.070 | 6.076-19.802 | 1.00 | 53.78 |
| 60 | ATOM | 213 | CG | PRO | A | 333 | 4.101 | 7.028-19.290 | 1.00 | 53.42 |
| | ATOM | 214 | C | PRO | A | 333 | 1.673 | 7.478-21.398 | 1.00 | 52.17 |

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|----|------|-----|-----|-----|---|-----|--------|---------------|------|-------|
| 5 | ATOM | 215 | O | PRO | A | 333 | 1.879 | 8.690-21.395 | 1.00 | 51.19 |
| | ATOM | 216 | N | THR | A | 334 | 0.457 | 6.956-21.532 | 1.00 | 52.26 |
| | ATOM | 217 | CA | THR | A | 334 | -0.724 | 7.802-21.687 | 1.00 | 54.21 |
| | ATOM | 218 | CB | THR | A | 334 | -1.997 | 6.949-21.813 | 1.00 | 53.90 |
| | ATOM | 219 | OG1 | THR | A | 334 | -1.971 | 6.256-23.065 | 1.00 | 53.92 |
| 10 | ATOM | 220 | CG2 | THR | A | 334 | -3.237 | 7.821-21.761 | 1.00 | 54.15 |
| | ATOM | 221 | C | THR | A | 334 | -0.864 | 8.782-20.525 | 1.00 | 56.34 |
| | ATOM | 222 | O | THR | A | 334 | -1.389 | 8.443-19.461 | 1.00 | 56.44 |
| | ATOM | 223 | N | ARG | A | 335 | -0.386 | 10.002-20.766 | 1.00 | 58.24 |
| | ATOM | 224 | CA | ARG | A | 335 | -0.377 | 11.099-19.801 | 1.00 | 57.96 |
| 15 | ATOM | 225 | CB | ARG | A | 335 | -0.569 | 12.427-20.531 | 1.00 | 60.22 |
| | ATOM | 226 | C | ARG | A | 335 | -1.349 | 10.996-18.627 | 1.00 | 56.61 |
| | ATOM | 227 | O | ARG | A | 335 | -0.919 | 10.908-17.475 | 1.00 | 60.70 |
| | ATOM | 228 | N | PRO | A | 336 | -2.667 | 11.015-18.889 | 1.00 | 52.43 |
| | ATOM | 229 | CD | PRO | A | 336 | -3.389 | 11.117-20.165 | 1.00 | 49.06 |
| 20 | ATOM | 230 | CA | PRO | A | 336 | -3.587 | 10.915-17.752 | 1.00 | 49.58 |
| | ATOM | 231 | CB | PRO | A | 336 | -4.911 | 11.456-18.302 | 1.00 | 48.66 |
| | ATOM | 232 | CG | PRO | A | 336 | -4.645 | 11.809-19.760 | 1.00 | 51.33 |
| | ATOM | 233 | C | PRO | A | 336 | -3.698 | 9.468-17.279 | 1.00 | 49.25 |
| | ATOM | 234 | O | PRO | A | 336 | -4.340 | 8.644-17.929 | 1.00 | 48.06 |
| 25 | ATOM | 235 | N | PHE | A | 337 | -3.063 | 9.170-16.147 | 1.00 | 47.90 |
| | ATOM | 236 | CA | PHE | A | 337 | -3.055 | 7.821-15.582 | 1.00 | 46.61 |
| | ATOM | 237 | CB | PHE | A | 337 | -2.063 | 7.732-14.421 | 1.00 | 47.73 |
| | ATOM | 238 | CG | PHE | A | 337 | -0.649 | 8.011-14.805 | 1.00 | 46.27 |
| | ATOM | 239 | CD1 | PHE | A | 337 | -0.017 | 9.168-14.368 | 1.00 | 46.55 |
| 30 | ATOM | 240 | CD2 | PHE | A | 337 | 0.061 | 7.113-15.591 | 1.00 | 48.12 |
| | ATOM | 241 | CE1 | PHE | A | 337 | 1.305 | 9.429-14.707 | 1.00 | 48.09 |
| | ATOM | 242 | CE2 | PHE | A | 337 | 1.386 | 7.364-15.938 | 1.00 | 47.57 |
| | ATOM | 243 | CZ | PHE | A | 337 | 2.009 | 8.525-15.495 | 1.00 | 48.40 |
| | ATOM | 244 | C | PHE | A | 337 | -4.401 | 7.338-15.071 | 1.00 | 46.15 |
| 35 | ATOM | 245 | O | PHE | A | 337 | -5.250 | 8.127-14.671 | 1.00 | 48.34 |
| | ATOM | 246 | N | SER | A | 338 | -4.573 | 6.022-15.080 | 1.00 | 45.06 |
| | ATOM | 247 | CA | SER | A | 338 | -5.781 | 5.385-14.578 | 1.00 | 45.12 |
| | ATOM | 248 | CB | SER | A | 338 | -6.477 | 4.594-15.684 | 1.00 | 44.49 |
| | ATOM | 249 | OG | SER | A | 338 | -6.227 | 3.206-15.554 | 1.00 | 45.78 |
| 40 | ATOM | 250 | C | SER | A | 338 | -5.292 | 4.439-13.488 | 1.00 | 47.04 |
| | ATOM | 251 | O | SER | A | 338 | -4.090 | 4.186-13.387 | 1.00 | 44.08 |
| | ATOM | 252 | N | GLU | A | 339 | -6.206 | 3.916-12.676 | 1.00 | 45.63 |
| | ATOM | 253 | CA | GLU | A | 339 | -5.802 | 3.012-11.608 | 1.00 | 45.40 |
| | ATOM | 254 | CB | GLU | A | 339 | -7.015 | 2.521-10.814 | 1.00 | 45.66 |
| 45 | ATOM | 255 | CG | GLU | A | 339 | -6.637 | 1.680 -9.600 | 1.00 | 46.81 |
| | ATOM | 256 | CD | GLU | A | 339 | -7.717 | 1.652 -8.535 | 1.00 | 47.56 |
| | ATOM | 257 | OE1 | GLU | A | 339 | -8.471 | 0.656 -8.477 | 1.00 | 47.37 |
| | ATOM | 258 | OE2 | GLU | A | 339 | -7.810 | 2.625 -7.754 | 1.00 | 49.29 |
| | ATOM | 259 | C | GLU | A | 339 | -5.040 | 1.821-12.170 | 1.00 | 45.23 |
| 50 | ATOM | 260 | O | GLU | A | 339 | -3.862 | 1.641-11.872 | 1.00 | 46.51 |
| | ATOM | 261 | N | ALA | A | 340 | -5.712 | 1.010-12.982 | 1.00 | 42.87 |
| | ATOM | 262 | CA | ALA | A | 340 | -5.078 | -0.158-13.574 | 1.00 | 40.24 |
| | ATOM | 263 | CB | ALA | A | 340 | -6.055 | -0.871-14.496 | 1.00 | 41.40 |
| | ATOM | 264 | C | ALA | A | 340 | -3.837 | 0.273-14.350 | 1.00 | 38.83 |
| 55 | ATOM | 265 | O | ALA | A | 340 | -2.909 | -0.515-14.543 | 1.00 | 35.58 |
| | ATOM | 266 | N | SER | A | 341 | -3.836 | 1.535-14.773 | 1.00 | 35.79 |
| | ATOM | 267 | CA | SER | A | 341 | -2.742 | 2.133-15.537 | 1.00 | 36.58 |
| | ATOM | 268 | CB | SER | A | 341 | -3.231 | 3.454-16.154 | 1.00 | 39.01 |
| | ATOM | 269 | OG | SER | A | 341 | -2.211 | 4.130-16.864 | 1.00 | 36.09 |
| 60 | ATOM | 270 | C | SER | A | 341 | -1.480 | 2.376-14.691 | 1.00 | 35.63 |
| | ATOM | 271 | O | SER | A | 341 | -0.389 | 1.913-15.038 | 1.00 | 33.20 |

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|----|------|-----|-----|-----|---|-----|--------|---------------|------|-------|
| 5 | ATOM | 272 | N | MET | A | 342 | -1.626 | 3.115-13.595 | 1.00 | 35.92 |
| | ATOM | 273 | CA | MET | A | 342 | -0.498 | 3.396-12.708 | 1.00 | 35.88 |
| | ATOM | 274 | CB | MET | A | 342 | -0.912 | 4.396-11.623 | 1.00 | 35.96 |
| | ATOM | 275 | CG | MET | A | 342 | 0.241 | 5.218-11.059 | 1.00 | 38.02 |
| | ATOM | 276 | SD | MET | A | 342 | -0.308 | 6.374 -9.780 | 1.00 | 44.73 |
| 10 | ATOM | 277 | CE | MET | A | 342 | 0.626 | 7.815-10.205 | 1.00 | 42.49 |
| | ATOM | 278 | C | MET | A | 342 | -0.011 | 2.100-12.059 | 1.00 | 34.17 |
| | ATOM | 279 | O | MET | A | 342 | 1.195 | 1.880-11.909 | 1.00 | 33.40 |
| | ATOM | 280 | N | MET | A | 343 | -0.957 | 1.243-11.687 | 1.00 | 29.95 |
| | ATOM | 281 | CA | MET | A | 343 | -0.640 | -0.034-11.062 | 1.00 | 31.96 |
| 15 | ATOM | 282 | CB | MET | A | 343 | -1.921 | -0.810-10.751 | 1.00 | 31.70 |
| | ATOM | 283 | CG | MET | A | 343 | -2.667 | -0.337 -9.502 | 1.00 | 37.13 |
| | ATOM | 284 | SD | MET | A | 343 | -1.749 | -0.507 -7.940 | 1.00 | 36.00 |
| | ATOM | 285 | CE | MET | A | 343 | -1.468 | -2.299 -7.886 | 1.00 | 32.14 |
| | ATOM | 286 | C | MET | A | 343 | 0.234 | -0.875-11.979 | 1.00 | 31.72 |
| 20 | ATOM | 287 | O | MET | A | 343 | 1.159 | -1.558-11.527 | 1.00 | 30.26 |
| | ATOM | 288 | N | GLY | A | 344 | -0.069 | -0.823-13.272 | 1.00 | 29.04 |
| | ATOM | 289 | CA | GLY | A | 344 | 0.688 | -1.591-14.242 | 1.00 | 24.94 |
| | ATOM | 290 | C | GLY | A | 344 | 2.104 | -1.085-14.396 | 1.00 | 26.01 |
| | ATOM | 291 | O | GLY | A | 344 | 3.046 | -1.873-14.463 | 1.00 | 28.72 |
| 25 | ATOM | 292 | N | LEU | A | 345 | 2.257 | 0.232-14.471 | 1.00 | 26.97 |
| | ATOM | 293 | CA | LEU | A | 345 | 3.576 | 0.839-14.608 | 1.00 | 31.15 |
| | ATOM | 294 | CB | LEU | A | 345 | 3.459 | 2.361-14.753 | 1.00 | 30.06 |
| | ATOM | 295 | CG | LEU | A | 345 | 2.765 | 2.924-15.995 | 1.00 | 33.50 |
| | ATOM | 296 | CD1 | LEU | A | 345 | 2.901 | 4.439-15.999 | 1.00 | 33.52 |
| 30 | ATOM | 297 | CD2 | LEU | A | 345 | 3.379 | 2.324-17.257 | 1.00 | 33.22 |
| | ATOM | 298 | C | LEU | A | 345 | 4.433 | 0.534-13.383 | 1.00 | 30.31 |
| | ATOM | 299 | O | LEU | A | 345 | 5.564 | 0.061-13.505 | 1.00 | 32.80 |
| | ATOM | 300 | N | LEU | A | 346 | 3.884 | 0.813-12.205 | 1.00 | 27.83 |
| | ATOM | 301 | CA | LEU | A | 346 | 4.595 | 0.596-10.947 | 1.00 | 26.19 |
| 35 | ATOM | 302 | CB | LEU | A | 346 | 3.729 | 1.063 -9.783 | 1.00 | 24.51 |
| | ATOM | 303 | CG | LEU | A | 346 | 3.483 | 2.569 -9.682 | 1.00 | 26.33 |
| | ATOM | 304 | CD1 | LEU | A | 346 | 2.623 | 2.844 -8.463 | 1.00 | 27.33 |
| | ATOM | 305 | CD2 | LEU | A | 346 | 4.809 | 3.317 -9.587 | 1.00 | 24.89 |
| | ATOM | 306 | C | LEU | A | 346 | 5.032 | -0.848-10.707 | 1.00 | 25.72 |
| 40 | ATOM | 307 | O | LEU | A | 346 | 6.181 | -1.102-10.345 | 1.00 | 29.86 |
| | ATOM | 308 | N | THR | A | 347 | 4.117 | -1.793-10.891 | 1.00 | 23.80 |
| | ATOM | 309 | CA | THR | A | 347 | 4.436 | -3.196-10.674 | 1.00 | 23.91 |
| | ATOM | 310 | CB | THR | A | 347 | 3.164 | -4.058-10.641 | 1.00 | 26.39 |
| | ATOM | 311 | OG1 | THR | A | 347 | 2.421 | -3.860-11.849 | 1.00 | 24.57 |
| 45 | ATOM | 312 | CG2 | THR | A | 347 | 2.301 | -3.682 -9.444 | 1.00 | 23.98 |
| | ATOM | 313 | C | THR | A | 347 | 5.366 | -3.734-11.756 | 1.00 | 26.17 |
| | ATOM | 314 | O | THR | A | 347 | 6.176 | -4.622-11.496 | 1.00 | 27.44 |
| | ATOM | 315 | N | ASN | A | 348 | 5.242 | -3.197-12.970 | 1.00 | 25.48 |
| | ATOM | 316 | CA | ASN | A | 348 | 6.092 | -3.617-14.082 | 1.00 | 23.77 |
| 50 | ATOM | 317 | CB | ASN | A | 348 | 5.657 | -2.926-15.385 | 1.00 | 24.59 |
| | ATOM | 318 | CG | ASN | A | 348 | 6.522 | -3.302-16.571 | 1.00 | 29.93 |
| | ATOM | 319 | OD1 | ASN | A | 348 | 7.616 | -2.799-16.771 | 1.00 | 24.81 |
| | ATOM | 320 | ND2 | ASN | A | 348 | 6.010 | -4.236-17.391 | 1.00 | 32.61 |
| | ATOM | 321 | C | ASN | A | 348 | 7.532 | -3.229-13.741 | 1.00 | 22.82 |
| 55 | ATOM | 322 | O | ASN | A | 348 | 8.453 | -4.027-13.870 | 1.00 | 18.83 |
| | ATOM | 323 | N | LEU | A | 349 | 7.711 | -1.993-13.288 | 1.00 | 22.58 |
| | ATOM | 324 | CA | LEU | A | 349 | 9.030 | -1.507-12.914 | 1.00 | 21.85 |
| | ATOM | 325 | CB | LEU | A | 349 | 8.929 | -0.028-12.536 | 1.00 | 22.00 |
| | ATOM | 326 | CG | LEU | A | 349 | 10.155 | 0.673-11.953 | 1.00 | 23.64 |
| 60 | ATOM | 327 | CD1 | LEU | A | 349 | 11.224 | 0.826-13.017 | 1.00 | 19.35 |
| | ATOM | 328 | CD2 | LEU | A | 349 | 9.726 | 2.040-11.415 | 1.00 | 21.97 |

| | | | | | | | | | | |
|----|------|-----|-----|-----|---|-----|--------|----------------|------|-------|
| 5 | ATOM | 329 | C | LEU | A | 349 | 9.564 | -2.335-11.734 | 1.00 | 22.94 |
| | ATOM | 330 | O | LEU | A | 349 | 10.724 | -2.749-11.717 | 1.00 | 23.97 |
| | ATOM | 331 | N | ALA | A | 350 | 8.705 | -2.591-10.756 | 1.00 | 21.67 |
| | ATOM | 332 | CA | ALA | A | 350 | 9.113 | -3.356 -9.586 | 1.00 | 21.83 |
| 10 | ATOM | 333 | CB | ALA | A | 350 | 7.963 | -3.441 -8.593 | 1.00 | 18.95 |
| | ATOM | 334 | C | ALA | A | 350 | 9.568 | -4.757 -9.985 | 1.00 | 21.90 |
| | ATOM | 335 | O | ALA | A | 350 | 10.625 | -5.221 -9.554 | 1.00 | 24.15 |
| | ATOM | 336 | N | ASP | A | 351 | 8.767 | -5.423-10.810 | 1.00 | 23.24 |
| 15 | ATOM | 337 | CA | ASP | A | 351 | 9.093 | -6.772-11.259 | 1.00 | 25.87 |
| | ATOM | 338 | CB | ASP | A | 351 | 8.028 | -7.274-12.239 | 1.00 | 27.03 |
| | ATOM | 339 | CG | ASP | A | 351 | 8.103 | -8.772-12.458 | 1.00 | 31.64 |
| | ATOM | 340 | OD1 | ASP | A | 351 | 8.217 | -9.196-13.628 | 1.00 | 35.06 |
| 20 | ATOM | 341 | OD2 | ASP | A | 351 | 8.049 | -9.525-11.464 | 1.00 | 36.86 |
| | ATOM | 342 | C | ASP | A | 351 | 10.469 | -6.825-11.912 | 1.00 | 22.36 |
| | ATOM | 343 | O | ASP | A | 351 | 11.219 | -7.773-11.702 | 1.00 | 25.15 |
| | ATOM | 344 | N | ARG | A | 352 | 10.810 | -5.808-12.697 | 1.00 | 23.58 |
| 25 | ATOM | 345 | CA | ARG | A | 352 | 12.115 | -5.787-13.347 | 1.00 | 21.07 |
| | ATOM | 346 | CB | ARG | A | 352 | 12.120 | -4.785-14.507 | 1.00 | 21.02 |
| | ATOM | 347 | CG | ARG | A | 352 | 11.539 | -5.352-15.797 | 1.00 | 20.44 |
| | ATOM | 348 | CD | ARG | A | 352 | 11.554 | -4.319-16.915 | 1.00 | 20.43 |
| 30 | ATOM | 349 | NE | ARG | A | 352 | 10.592 | -3.245-16.687 | 1.00 | 19.85 |
| | ATOM | 350 | CZ | ARG | A | 352 | 10.910 | -1.954-16.641 | 1.00 | 19.69 |
| | ATOM | 351 | NH1 | ARG | A | 352 | 12.172 | -1.564-16.813 | 1.00 | 17.36 |
| | ATOM | 352 | NH2 | ARG | A | 352 | 9.962 | -1.049-16.441 | 1.00 | 21.88 |
| 35 | ATOM | 353 | C | ARG | A | 352 | 13.223 | -5.442-12.350 | 1.00 | 22.11 |
| | ATOM | 354 | O | ARG | A | 352 | 14.346 | -5.945-12.454 | 1.00 | 24.13 |
| | ATOM | 355 | N | GLU | A | 353 | 12.909 | -4.587-11.383 | 1.00 | 18.66 |
| | ATOM | 356 | CA | GLU | A | 353 | 13.888 | -4.206-10.376 | 1.00 | 19.08 |
| 40 | ATOM | 357 | CB | GLU | A | 353 | 13.317 | -3.102 -9.483 | 1.00 | 21.62 |
| | ATOM | 358 | CG | GLU | A | 353 | 13.295 | -1.718-10.114 | 1.00 | 20.97 |
| | ATOM | 359 | CD | GLU | A | 353 | 12.832 | -0.648 -9.129 | 1.00 | 23.84 |
| | ATOM | 360 | OE1 | GLU | A | 353 | 11.611 | -0.531 -8.926 | 1.00 | 24.76 |
| 45 | ATOM | 361 | OE2 | GLU | A | 353 | 13.686 | 0.066 -8.557 | 1.00 | 24.95 |
| | ATOM | 362 | C | GLU | A | 353 | 14.246 | -5.423 -9.512 | 1.00 | 20.14 |
| | ATOM | 363 | O | GLU | A | 353 | 15.398 | -5.600 -9.104 | 1.00 | 19.40 |
| | ATOM | 364 | N | LEU | A | 354 | 13.246 | -6.257 -9.235 | 1.00 | 19.54 |
| 50 | ATOM | 365 | CA | LEU | A | 354 | 13.434 | -7.452 -8.415 | 1.00 | 21.77 |
| | ATOM | 366 | CB | LEU | A | 354 | 12.107 | -8.209 -8.270 | 1.00 | 23.09 |
| | ATOM | 367 | CG | LEU | A | 354 | 11.160 | -7.606 -7.223 | 1.00 | 25.00 |
| | ATOM | 368 | CD1 | LEU | A | 354 | 9.720 | -8.013 -7.510 | 1.00 | 23.49 |
| 55 | ATOM | 369 | CD2 | LEU | A | 354 | 11.584 | -8.069 -5.839 | 1.00 | 23.31 |
| | ATOM | 370 | C | LEU | A | 354 | 14.500 | -8.386 -8.981 | 1.00 | 23.21 |
| | ATOM | 371 | O | LEU | A | 354 | 15.255 | -9.007 -8.234 | 1.00 | 22.44 |
| | ATOM | 372 | N | VAL | A | 355 | 14.560 | -8.490-10.302 | 1.00 | 22.52 |
| 60 | ATOM | 373 | CA | VAL | A | 355 | 15.551 | -9.343-10.935 | 1.00 | 21.66 |
| | ATOM | 374 | CB | VAL | A | 355 | 15.353 | -9.365-12.466 | 1.00 | 24.35 |
| | ATOM | 375 | CG1 | VAL | A | 355 | 16.435 | -10.214-13.119 | 1.00 | 28.16 |
| | ATOM | 376 | CG2 | VAL | A | 355 | 13.957 | -9.886-12.798 | 1.00 | 21.59 |
| 65 | ATOM | 377 | C | VAL | A | 355 | 16.944 | -8.811-10.606 | 1.00 | 23.74 |
| | ATOM | 378 | O | VAL | A | 355 | 17.857 | -9.581-10.291 | 1.00 | 23.51 |
| | ATOM | 379 | N | HIS | A | 356 | 17.105 | -7.489-10.669 | 1.00 | 21.27 |
| | ATOM | 380 | CA | HIS | A | 356 | 18.392 | -6.861-10.369 | 1.00 | 21.31 |
| 70 | ATOM | 381 | CB | HIS | A | 356 | 18.384 | -5.390-10.811 | 1.00 | 19.87 |
| | ATOM | 382 | CG | HIS | A | 356 | 18.494 | -5.205-12.295 | 1.00 | 21.77 |
| | ATOM | 383 | CD2 | HIS | A | 356 | 17.543 | -5.048-13.248 | 1.00 | 21.66 |
| | ATOM | 384 | ND1 | HIS | A | 356 | 19.704 | -5.177-12.955 | 1.00 | 21.11 |
| 75 | ATOM | 385 | CE1 | HIS | A | 356 | 19.496 | -5.011-14.249 | 1.00 | 24.96 |
| | ATOM | | | | | | | | | |

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|----|------|-----|-----|------|---|-----|--------|---------|---------|------|-------|
| 5 | ATOM | 386 | NE2 | HIS | A | 356 | 18.192 | -4.931 | -14.455 | 1.00 | 18.37 |
| | ATOM | 387 | C | HIS | A | 356 | 18.702 | -6.947 | -8.875 | 1.00 | 21.41 |
| | ATOM | 388 | O | HIS | A | 356 | 19.864 | -7.111 | -8.465 | 1.00 | 21.88 |
| | ATOM | 389 | N | MET | A | 357 | 17.660 | -6.843 | -8.058 | 1.00 | 21.84 |
| | ATOM | 390 | CA | MET | A | 357 | 17.837 | -6.906 | -6.610 | 1.00 | 21.51 |
| 10 | ATOM | 391 | CB | MET | A | 357 | 16.503 | -6.668 | -5.898 | 1.00 | 17.60 |
| | ATOM | 392 | CG | MET | A | 357 | 16.629 | -6.579 | -4.369 | 1.00 | 19.36 |
| | ATOM | 393 | SD | MET | A | 357 | 15.051 | -6.755 | -3.531 | 1.00 | 23.64 |
| | ATOM | 394 | CE | MET | A | 357 | 14.189 | -5.332 | -4.163 | 1.00 | 23.13 |
| | ATOM | 395 | C | MET | A | 357 | 18.411 | -8.259 | -6.192 | 1.00 | 23.69 |
| 15 | ATOM | 396 | O | MET | A | 357 | 19.337 | -8.328 | -5.389 | 1.00 | 24.41 |
| | ATOM | 397 | N | ILE | A | 358 | 17.856 | -9.331 | -6.746 | 1.00 | 27.14 |
| | ATOM | 398 | CA | ILE | A | 358 | 18.314 | -10.672 | -6.425 | 1.00 | 28.79 |
| | ATOM | 399 | CB | ILE | A | 358 | 17.529 | -11.725 | -7.232 | 1.00 | 32.42 |
| | ATOM | 400 | CG2 | ILE | A | 358 | 18.267 | -13.064 | -7.220 | 1.00 | 32.77 |
| 20 | ATOM | 401 | CG1 | ILE | A | 358 | 16.125 | -11.880 | -6.644 | 1.00 | 31.94 |
| | ATOM | 402 | CD1 | ILE | A | 358 | 15.062 | -12.196 | -7.680 | 1.00 | 34.85 |
| | ATOM | 403 | C | ILE | A | 358 | 19.801 | -10.802 | -6.728 | 1.00 | 28.75 |
| | ATOM | 404 | O | ILE | A | 358 | 20.569 | -11.305 | -5.912 | 1.00 | 31.60 |
| | ATOM | 405 | N | ASN | A | 359 | 20.207 | -10.325 | -7.897 | 1.00 | 27.91 |
| 25 | ATOM | 406 | CA | ASN | A | 359 | 21.601 | -10.401 | -8.293 | 1.00 | 29.16 |
| | ATOM | 407 | CB | ASN | A | 359 | 21.721 | -10.172 | -9.801 | 1.00 | 31.88 |
| | ATOM | 408 | CG | ASN | A | 359 | 21.253 | -11.381 | -10.599 | 1.00 | 39.34 |
| | ATOM | 409 | OD1 | ASN | A | 359 | 21.916 | -12.422 | -10.612 | 1.00 | 41.27 |
| | ATOM | 410 | ND2 | ASN | A | 359 | 20.102 | -11.255 | -11.253 | 1.00 | 38.58 |
| 30 | ATOM | 411 | C | ASN | A | 359 | 22.476 | -9.436 | -7.510 | 1.00 | 30.75 |
| | ATOM | 412 | O | ASN | A | 359 | 23.686 | -9.629 | -7.412 | 1.00 | 33.35 |
| | ATOM | 413 | N | TRP | A | 360 | 21.872 | -8.400 | -6.940 | 1.00 | 30.07 |
| | ATOM | 414 | CA | TRP | A | 360 | 22.634 | -7.451 | -6.132 | 1.00 | 27.87 |
| | ATOM | 415 | CB | TRP | A | 360 | 21.849 | -6.150 | -5.948 | 1.00 | 24.80 |
| 35 | ATOM | 416 | CG | TRP | A | 360 | 22.196 | -5.392 | -4.691 | 1.00 | 23.04 |
| | ATOM | 417 | CD2 | TRP | A | 360 | 21.501 | -5.443 | -3.438 | 1.00 | 19.83 |
| | ATOM | 418 | CE2 | TRP | A | 360 | 22.147 | -4.543 | -2.564 | 1.00 | 22.31 |
| | ATOM | 419 | CE3 | TRP | A | 360 | 20.392 | -6.165 | -2.972 | 1.00 | 20.09 |
| | ATOM | 420 | CD1 | TRP | A | 360 | 23.212 | -4.488 | -4.529 | 1.00 | 18.99 |
| 40 | ATOM | 421 | NE1 | TRP | A | 360 | 23.187 | -3.974 | -3.255 | 1.00 | 21.17 |
| | ATOM | 422 | CZ2 | TRP | A | 360 | 21.721 | -4.340 | -1.243 | 1.00 | 20.43 |
| | ATOM | 423 | CZ3 | TRP | A | 360 | 19.968 | -5.965 | -1.661 | 1.00 | 20.12 |
| | ATOM | 424 | CH2 | TRP | A | 360 | 20.635 | -5.057 | -0.812 | 1.00 | 18.54 |
| | ATOM | 425 | C | TRP | A | 360 | 22.892 | -8.099 | -4.766 | 1.00 | 24.88 |
| 45 | ATOM | 426 | O | TRP | A | 360 | 23.978 | -7.980 | -4.198 | 1.00 | 25.00 |
| | ATOM | 427 | N | ALA | A | 361 | 21.879 | -8.789 | -4.252 | 1.00 | 24.08 |
| | ATOM | 428 | CA | ALA | A | 361 | 21.972 | -9.462 | -2.958 | 1.00 | 26.06 |
| | ATOM | 429 | CB | ALA | A | 361 | 20.676 | -10.203 | -2.672 | 1.00 | 20.27 |
| | ATOM | 430 | C | ALA | A | 361 | 23.161 | -10.433 | -2.897 | 1.00 | 28.44 |
| 50 | ATOM | 431 | O | ALA | A | 361 | 23.843 | -10.531 | -1.876 | 1.00 | 28.95 |
| | ATOM | 432 | N | LYS | A | 362 | 23.414 | -11.144 | -3.992 | 1.00 | 31.41 |
| | ATOM | 433 | CA | LYS | A | 362 | 24.530 | -12.097 | -4.047 | 1.00 | 33.33 |
| | ATOM | 434 | CB | LYS | A | 362 | 24.564 | -12.824 | -5.390 | 1.00 | 34.81 |
| | ATOM | 435 | CG | LYS | A | 362 | 23.319 | -13.608 | -5.756 | 1.00 | 36.27 |
| 55 | ATOM | 436 | CD | LYS | A | 362 | 23.458 | -14.178 | -7.167 | 1.00 | 38.30 |
| | ATOM | 437 | CE | LYS | A | 362 | 22.369 | -15.193 | -7.472 | 1.00 | 40.94 |
| | ATOM | 438 | NZ | LYS | A | 362 | 22.111 | -15.322 | -8.937 | 1.00 | 42.49 |
| | ATOM | 439 | C | LYS | A | 362 | 25.854 | -11.351 | -3.893 | 1.00 | 34.17 |
| | ATOM | 440 | O | LYS | A | 362 | 26.880 | -11.977 | -3.595 | 1.00 | 35.40 |
| 60 | ATOM | 441 | N | AARG | A | 363 | 25.826 | -10.059 | -4.095 | 0.50 | 34.23 |
| | ATOM | 442 | N | BARG | A | 363 | 25.826 | -10.059 | -4.095 | 0.50 | 34.03 |

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|----|------|-----|-----|------|---|-----|--------|---------|---------|------|-------|
| 5 | ATOM | 443 | CA | AARG | A | 363 | 27.035 | -9.254 | -3.987 | 0.50 | 33.25 |
| | ATOM | 444 | CA | BARG | A | 363 | 27.035 | -9.254 | -3.987 | 0.50 | 32.83 |
| | ATOM | 445 | CB | AARG | A | 363 | 27.031 | -8.153 | -5.044 | 0.50 | 34.67 |
| | ATOM | 446 | CB | BARG | A | 363 | 27.031 | -8.153 | -5.045 | 0.50 | 34.20 |
| | ATOM | 447 | CG | AARG | A | 363 | 26.933 | -8.654 | -6.478 | 0.50 | 36.32 |
| 10 | ATOM | 448 | CG | BARG | A | 363 | 26.930 | -8.654 | -6.480 | 0.50 | 35.56 |
| | ATOM | 449 | CD | AARG | A | 363 | 27.745 | -7.775 | -7.415 | 0.50 | 38.39 |
| | ATOM | 450 | CD | BARG | A | 363 | 27.752 | -7.781 | -7.414 | 0.50 | 37.18 |
| | ATOM | 451 | NE | AARG | A | 363 | 29.171 | -7.793 | -7.091 | 0.50 | 39.98 |
| | ATOM | 452 | NE | BARG | A | 363 | 27.195 | -7.725 | -8.762 | 0.50 | 37.39 |
| 15 | ATOM | 453 | CZ | AARG | A | 363 | 30.086 | -7.038 | -7.692 | 0.50 | 40.54 |
| | ATOM | 454 | CZ | BARG | A | 363 | 27.905 | -7.457 | -9.855 | 0.50 | 40.02 |
| | ATOM | 455 | NH1 | AARG | A | 363 | 29.735 | -6.218 | -8.675 | 0.50 | 38.13 |
| | ATOM | 456 | NH1 | BARG | A | 363 | 29.205 | -7.191 | -9.761 | 0.50 | 40.42 |
| | ATOM | 457 | NH2 | AARG | A | 363 | 31.358 | -7.123 | -7.326 | 0.50 | 43.19 |
| 20 | ATOM | 458 | NH2 | BARG | A | 363 | 27.311 | -7.436 | -11.041 | 0.50 | 38.91 |
| | ATOM | 459 | C | AARG | A | 363 | 27.207 | -8.630 | -2.610 | 0.50 | 33.28 |
| | ATOM | 460 | C | BARG | A | 363 | 27.207 | -8.630 | -2.610 | 0.50 | 32.81 |
| | ATOM | 461 | O | AARG | A | 363 | 28.223 | -7.992 | -2.344 | 0.50 | 34.18 |
| | ATOM | 462 | O | BARG | A | 363 | 28.223 | -7.992 | -2.345 | 0.50 | 33.43 |
| 25 | ATOM | 463 | N | VAL | A | 364 | 26.215 | -8.798 | -1.740 | 1.00 | 33.12 |
| | ATOM | 464 | CA | VAL | A | 364 | 26.288 | -8.240 | -0.389 | 1.00 | 33.63 |
| | ATOM | 465 | CB | VAL | A | 364 | 24.898 | -8.178 | 0.292 | 1.00 | 34.97 |
| | ATOM | 466 | CG1 | VAL | A | 364 | 25.036 | -7.608 | 1.700 | 1.00 | 35.44 |
| | ATOM | 467 | CG2 | VAL | A | 364 | 23.946 | -7.328 | -0.532 | 1.00 | 36.69 |
| 30 | ATOM | 468 | C | VAL | A | 364 | 27.184 | -9.157 | 0.428 | 1.00 | 34.27 |
| | ATOM | 469 | O | VAL | A | 364 | 26.878 | -10.341 | 0.603 | 1.00 | 34.95 |
| | ATOM | 470 | N | PRO | A | 365 | 28.306 | -8.626 | 0.935 | 1.00 | 36.08 |
| | ATOM | 471 | CD | PRO | A | 365 | 28.775 | -7.235 | 0.793 | 1.00 | 34.84 |
| | ATOM | 472 | CA | PRO | A | 365 | 29.231 | -9.442 | 1.733 | 1.00 | 37.82 |
| 35 | ATOM | 473 | CB | PRO | A | 365 | 30.110 | -8.408 | 2.430 | 1.00 | 34.31 |
| | ATOM | 474 | CG | PRO | A | 365 | 30.127 | -7.247 | 1.475 | 1.00 | 37.77 |
| | ATOM | 475 | C | PRO | A | 365 | 28.538 | -10.373 | 2.720 | 1.00 | 37.61 |
| | ATOM | 476 | O | PRO | A | 365 | 27.692 | -9.945 | 3.507 | 1.00 | 37.74 |
| | ATOM | 477 | N | GLY | A | 366 | 28.890 | -11.654 | 2.654 | 1.00 | 39.04 |
| 40 | ATOM | 478 | CA | GLY | A | 366 | 28.307 | -12.635 | 3.554 | 1.00 | 38.27 |
| | ATOM | 479 | C | GLY | A | 366 | 26.991 | -13.264 | 3.138 | 1.00 | 39.32 |
| | ATOM | 480 | O | GLY | A | 366 | 26.638 | -14.336 | 3.635 | 1.00 | 39.53 |
| | ATOM | 481 | N | PHE | A | 367 | 26.246 | -12.615 | 2.236 | 1.00 | 38.60 |
| | ATOM | 482 | CA | PHE | A | 367 | 24.960 | -13.148 | 1.783 | 1.00 | 36.36 |
| 45 | ATOM | 483 | CB | PHE | A | 367 | 24.281 | -12.178 | 0.808 | 1.00 | 32.10 |
| | ATOM | 484 | CG | PHE | A | 367 | 22.827 | -12.473 | 0.581 | 1.00 | 30.12 |
| | ATOM | 485 | CD1 | PHE | A | 367 | 22.401 | -13.083 | -0.596 | 1.00 | 28.95 |
| | ATOM | 486 | CD2 | PHE | A | 367 | 21.882 | -12.176 | 1.563 | 1.00 | 26.18 |
| | ATOM | 487 | CE1 | PHE | A | 367 | 21.050 | -13.400 | -0.792 | 1.00 | 29.42 |
| 50 | ATOM | 488 | CE2 | PHE | A | 367 | 20.535 | -12.491 | 1.373 | 1.00 | 27.60 |
| | ATOM | 489 | CZ | PHE | A | 367 | 20.118 | -13.103 | 0.196 | 1.00 | 26.81 |
| | ATOM | 490 | C | PHE | A | 367 | 25.072 | -14.519 | 1.117 | 1.00 | 36.82 |
| | ATOM | 491 | O | PHE | A | 367 | 24.244 | -15.398 | 1.359 | 1.00 | 36.55 |
| | ATOM | 492 | N | VAL | A | 368 | 26.088 | -14.694 | 0.276 | 1.00 | 38.28 |
| 55 | ATOM | 493 | CA | VAL | A | 368 | 26.289 | -15.965 | -0.420 | 1.00 | 42.34 |
| | ATOM | 494 | CB | VAL | A | 368 | 27.386 | -15.850 | -1.504 | 1.00 | 41.78 |
| | ATOM | 495 | CG1 | VAL | A | 368 | 26.972 | -14.831 | -2.550 | 1.00 | 44.60 |
| | ATOM | 496 | CG2 | VAL | A | 368 | 28.707 | -15.457 | -0.873 | 1.00 | 42.23 |
| | ATOM | 497 | C | VAL | A | 368 | 26.664 | -17.100 | 0.533 | 1.00 | 43.85 |
| 60 | ATOM | 498 | O | VAL | A | 368 | 26.469 | -18.274 | 0.216 | 1.00 | 44.85 |
| | ATOM | 499 | N | ASP | A | 369 | 27.199 | -16.750 | 1.699 | 1.00 | 44.93 |

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|----|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 500 | CA | ASP | A | 369 | 27.579 | -17.755 | 2.688 | 1.00 | 44.96 |
| | ATOM | 501 | CB | ASP | A | 369 | 28.336 | -17.106 | 3.849 | 1.00 | 43.76 |
| | ATOM | 502 | CG | ASP | A | 369 | 29.608 | -16.413 | 3.404 | 1.00 | 43.04 |
| | ATOM | 503 | OD1 | ASP | A | 369 | 30.121 | -15.570 | 4.167 | 1.00 | 44.32 |
| | ATOM | 504 | OD2 | ASP | A | 369 | 30.097 | -16.709 | 2.293 | 1.00 | 46.76 |
| 10 | ATOM | 505 | C | ASP | A | 369 | 26.340 | -18.465 | 3.228 | 1.00 | 45.89 |
| | ATOM | 506 | O | ASP | A | 369 | 26.360 | -19.671 | 3.475 | 1.00 | 48.61 |
| | ATOM | 507 | N | LEU | A | 370 | 25.261 | -17.714 | 3.407 | 1.00 | 43.59 |
| | ATOM | 508 | CA | LEU | A | 370 | 24.020 | -18.279 | 3.924 | 1.00 | 44.24 |
| | ATOM | 509 | CB | LEU | A | 370 | 22.980 | -17.173 | 4.110 | 1.00 | 41.42 |
| 15 | ATOM | 510 | CG | LEU | A | 370 | 23.404 | -16.015 | 5.014 | 1.00 | 41.45 |
| | ATOM | 511 | CD1 | LEU | A | 370 | 22.219 | -15.095 | 5.245 | 1.00 | 42.25 |
| | ATOM | 512 | CD2 | LEU | A | 370 | 23.931 | -16.552 | 6.332 | 1.00 | 38.35 |
| | ATOM | 513 | C | LEU | A | 370 | 23.449 | -19.360 | 3.013 | 1.00 | 44.03 |
| | ATOM | 514 | O | LEU | A | 370 | 23.773 | -19.423 | 1.829 | 1.00 | 43.63 |
| 20 | ATOM | 515 | N | THR | A | 371 | 22.593 | -20.206 | 3.575 | 1.00 | 44.29 |
| | ATOM | 516 | CA | THR | A | 371 | 21.968 | -21.272 | 2.806 | 1.00 | 44.84 |
| | ATOM | 517 | CB | THR | A | 371 | 21.293 | -22.302 | 3.730 | 1.00 | 45.65 |
| | ATOM | 518 | OG1 | THR | A | 371 | 20.262 | -21.663 | 4.495 | 1.00 | 46.43 |
| | ATOM | 519 | CG2 | THR | A | 371 | 22.314 | -22.903 | 4.677 | 1.00 | 46.48 |
| 25 | ATOM | 520 | C | THR | A | 371 | 20.923 | -20.684 | 1.864 | 1.00 | 44.93 |
| | ATOM | 521 | O | THR | A | 371 | 20.418 | -19.585 | 2.092 | 1.00 | 44.36 |
| | ATOM | 522 | N | LEU | A | 372 | 20.607 | -21.418 | 0.804 | 1.00 | 43.83 |
| | ATOM | 523 | CA | LEU | A | 372 | 19.624 | -20.971 | -0.166 | 1.00 | 44.62 |
| | ATOM | 524 | CB | LEU | A | 372 | 19.407 | -22.043 | -1.237 | 1.00 | 47.17 |
| 30 | ATOM | 525 | CG | LEU | A | 372 | 18.512 | -21.690 | -2.429 | 1.00 | 46.91 |
| | ATOM | 526 | CD1 | LEU | A | 372 | 19.005 | -20.417 | -3.098 | 1.00 | 48.73 |
| | ATOM | 527 | CD2 | LEU | A | 372 | 18.521 | -22.844 | -3.420 | 1.00 | 51.12 |
| | ATOM | 528 | C | LEU | A | 372 | 18.307 | -20.644 | 0.512 | 1.00 | 44.84 |
| | ATOM | 529 | O | LEU | A | 372 | 17.705 | -19.602 | 0.261 | 1.00 | 43.25 |
| 35 | ATOM | 530 | N | HIS | A | 373 | 17.849 | -21.558 | 1.382 | 1.00 | 43.14 |
| | ATOM | 531 | CA | HIS | A | 373 | 16.599 | -21.353 | 2.100 | 1.00 | 42.23 |
| | ATOM | 532 | CB | HIS | A | 373 | 16.318 | -22.525 | 3.062 | 1.00 | 45.38 |
| | ATOM | 533 | CG | HIS | A | 373 | 15.114 | -22.315 | 3.934 | 1.00 | 51.43 |
| | ATOM | 534 | CD2 | HIS | A | 373 | 13.808 | -22.621 | 3.743 | 1.00 | 54.99 |
| 40 | ATOM | 535 | ND1 | HIS | A | 373 | 15.187 | -21.716 | 5.174 | 1.00 | 54.26 |
| | ATOM | 536 | CE1 | HIS | A | 373 | 13.979 | -21.663 | 5.709 | 1.00 | 53.77 |
| | ATOM | 537 | NE2 | HIS | A | 373 | 13.124 | -22.206 | 4.861 | 1.00 | 55.27 |
| | ATOM | 538 | C | HIS | A | 373 | 16.665 | -20.047 | 2.885 | 1.00 | 39.78 |
| | ATOM | 539 | O | HIS | A | 373 | 15.677 | -19.324 | 2.971 | 1.00 | 37.71 |
| 45 | ATOM | 540 | N | ASP | A | 374 | 17.839 | -19.738 | 3.440 | 1.00 | 36.38 |
| | ATOM | 541 | CA | ASP | A | 374 | 18.020 | -18.516 | 4.219 | 1.00 | 37.21 |
| | ATOM | 542 | CB | ASP | A | 374 | 19.287 | -18.620 | 5.073 | 1.00 | 38.17 |
| | ATOM | 543 | CG | ASP | A | 374 | 19.064 | -19.425 | 6.344 | 1.00 | 41.47 |
| | ATOM | 544 | OD1 | ASP | A | 374 | 17.896 | -19.543 | 6.772 | 1.00 | 37.09 |
| 50 | ATOM | 545 | OD2 | ASP | A | 374 | 20.052 | -19.940 | 6.912 | 1.00 | 44.40 |
| | ATOM | 546 | C | ASP | A | 374 | 18.083 | -17.277 | 3.326 | 1.00 | 37.19 |
| | ATOM | 547 | O | ASP | A | 374 | 17.598 | -16.208 | 3.696 | 1.00 | 38.13 |
| | ATOM | 548 | N | GLN | A | 375 | 18.688 | -17.431 | 2.152 | 1.00 | 33.13 |
| | ATOM | 549 | CA | GLN | A | 375 | 18.788 | -16.339 | 1.198 | 1.00 | 31.94 |
| 55 | ATOM | 550 | CB | GLN | A | 375 | 19.634 | -16.756 | -0.001 | 1.00 | 28.81 |
| | ATOM | 551 | CG | GLN | A | 375 | 21.125 | -16.570 | 0.189 | 1.00 | 31.71 |
| | ATOM | 552 | CD | GLN | A | 375 | 21.920 | -17.222 | -0.922 | 1.00 | 34.49 |
| | ATOM | 553 | OE1 | GLN | A | 375 | 21.478 | -17.267 | -2.067 | 1.00 | 36.09 |
| | ATOM | 554 | NE2 | GLN | A | 375 | 23.097 | -17.736 | -0.588 | 1.00 | 40.32 |
| 60 | ATOM | 555 | C | GLN | A | 375 | 17.379 | -16.009 | 0.730 | 1.00 | 31.50 |
| | ATOM | 556 | O | GLN | A | 375 | 16.990 | -14.840 | 0.653 | 1.00 | 27.42 |

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|----|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 557 | N | VAL | A | 376 | 16.617 | -17.056 | 0.429 | 1.00 | 30.38 |
| | ATOM | 558 | CA | VAL | A | 376 | 15.242 | -16.907 | -0.027 | 1.00 | 33.50 |
| | ATOM | 559 | CB | VAL | A | 376 | 14.588 | -18.286 | -0.286 | 1.00 | 30.57 |
| | ATOM | 560 | CG1 | VAL | A | 376 | 13.093 | -18.122 | -0.516 | 1.00 | 33.14 |
| | ATOM | 561 | CG2 | VAL | A | 376 | 15.232 | -18.952 | -1.485 | 1.00 | 30.79 |
| 10 | ATOM | 562 | C | VAL | A | 376 | 14.393 | -16.159 | 1.002 | 1.00 | 33.80 |
| | ATOM | 563 | O | VAL | A | 376 | 13.653 | -15.237 | 0.661 | 1.00 | 34.89 |
| | ATOM | 564 | N | HIS | A | 377 | 14.500 | -16.568 | 2.261 | 1.00 | 33.35 |
| | ATOM | 565 | CA | HIS | A | 377 | 13.730 | -15.941 | 3.329 | 1.00 | 32.81 |
| | ATOM | 566 | CB | HIS | A | 377 | 13.966 | -16.694 | 4.644 | 1.00 | 35.24 |
| 15 | ATOM | 567 | CG | HIS | A | 377 | 13.429 | -15.989 | 5.851 | 1.00 | 40.15 |
| | ATOM | 568 | CD2 | HIS | A | 377 | 14.054 | -15.495 | 6.946 | 1.00 | 40.86 |
| | ATOM | 569 | ND1 | HIS | A | 377 | 12.090 | -15.703 | 6.012 | 1.00 | 43.08 |
| | ATOM | 570 | CE1 | HIS | A | 377 | 11.913 | -15.062 | 7.154 | 1.00 | 42.44 |
| | ATOM | 571 | NE2 | HIS | A | 377 | 13.089 | -14.922 | 7.740 | 1.00 | 44.85 |
| 20 | ATOM | 572 | C | HIS | A | 377 | 14.058 | -14.454 | 3.507 | 1.00 | 28.63 |
| | ATOM | 573 | O | HIS | A | 377 | 13.158 | -13.619 | 3.613 | 1.00 | 29.20 |
| | ATOM | 574 | N | LEU | A | 378 | 15.343 | -14.125 | 3.544 | 1.00 | 24.41 |
| | ATOM | 575 | CA | LEU | A | 378 | 15.759 | -12.738 | 3.721 | 1.00 | 23.21 |
| | ATOM | 576 | CB | LEU | A | 378 | 17.289 | -12.650 | 3.743 | 1.00 | 20.98 |
| 25 | ATOM | 577 | CG | LEU | A | 378 | 17.960 | -13.190 | 5.016 | 1.00 | 24.22 |
| | ATOM | 578 | CD1 | LEU | A | 378 | 19.471 | -13.041 | 4.924 | 1.00 | 21.07 |
| | ATOM | 579 | CD2 | LEU | A | 378 | 17.431 | -12.446 | 6.221 | 1.00 | 20.24 |
| | ATOM | 580 | C | LEU | A | 378 | 15.190 | -11.827 | 2.630 | 1.00 | 24.78 |
| | ATOM | 581 | O | LEU | A | 378 | 14.638 | -10.766 | 2.922 | 1.00 | 22.09 |
| 30 | ATOM | 582 | N | LEU | A | 379 | 15.321 | -12.242 | 1.374 | 1.00 | 24.13 |
| | ATOM | 583 | CA | LEU | A | 379 | 14.812 | -11.447 | 0.262 | 1.00 | 25.02 |
| | ATOM | 584 | CB | LEU | A | 379 | 15.307 | -12.025 | -1.062 | 1.00 | 27.12 |
| | ATOM | 585 | CG | LEU | A | 379 | 16.724 | -11.600 | -1.437 | 1.00 | 24.39 |
| | ATOM | 586 | CD1 | LEU | A | 379 | 17.299 | -12.557 | -2.470 | 1.00 | 27.58 |
| 35 | ATOM | 587 | CD2 | LEU | A | 379 | 16.679 | -10.178 | -1.983 | 1.00 | 29.05 |
| | ATOM | 588 | C | LEU | A | 379 | 13.287 | -11.355 | 0.246 | 1.00 | 27.61 |
| | ATOM | 589 | O | LEU | A | 379 | 12.726 | -10.301 | -0.062 | 1.00 | 26.16 |
| | ATOM | 590 | N | GLU | A | 380 | 12.616 | -12.454 | 0.576 | 1.00 | 25.65 |
| | ATOM | 591 | CA | GLU | A | 380 | 11.154 | -12.471 | 0.592 | 1.00 | 26.85 |
| 40 | ATOM | 592 | CB | GLU | A | 380 | 10.640 | -13.882 | 0.871 | 1.00 | 29.38 |
| | ATOM | 593 | CG | GLU | A | 380 | 10.718 | -14.796 | -0.331 | 1.00 | 35.58 |
| | ATOM | 594 | CD | GLU | A | 380 | 10.228 | -16.194 | -0.025 | 1.00 | 39.31 |
| | ATOM | 595 | OE1 | GLU | A | 380 | 10.142 | -17.008 | -0.967 | 1.00 | 42.89 |
| | ATOM | 596 | OE2 | GLU | A | 380 | 9.927 | -16.478 | 1.153 | 1.00 | 39.45 |
| 45 | ATOM | 597 | C | GLU | A | 380 | 10.604 | -11.526 | 1.649 | 1.00 | 25.43 |
| | ATOM | 598 | O | GLU | A | 380 | 9.551 | -10.925 | 1.469 | 1.00 | 27.75 |
| | ATOM | 599 | N | CYS | A | 381 | 11.324 | -11.400 | 2.753 | 1.00 | 25.57 |
| | ATOM | 600 | CA | CYS | A | 381 | 10.907 | -10.530 | 3.843 | 1.00 | 26.46 |
| | ATOM | 601 | CB | CYS | A | 381 | 11.570 | -11.000 | 5.149 | 1.00 | 31.46 |
| 50 | ATOM | 602 | SG | CYS | A | 381 | 11.305 | -9.946 | 6.623 | 1.00 | 45.32 |
| | ATOM | 603 | C | CYS | A | 381 | 11.262 | -9.059 | 3.589 | 1.00 | 24.77 |
| | ATOM | 604 | O | CYS | A | 381 | 10.516 | -8.166 | 3.975 | 1.00 | 25.01 |
| | ATOM | 605 | N | ALA | A | 382 | 12.377 | -8.815 | 2.903 | 1.00 | 22.23 |
| | ATOM | 606 | CA | ALA | A | 382 | 12.855 | -7.449 | 2.681 | 1.00 | 21.83 |
| 55 | ATOM | 607 | CB | ALA | A | 382 | 14.319 | -7.383 | 3.095 | 1.00 | 21.56 |
| | ATOM | 608 | C | ALA | A | 382 | 12.705 | -6.778 | 1.311 | 1.00 | 19.78 |
| | ATOM | 609 | O | ALA | A | 382 | 12.996 | -5.587 | 1.182 | 1.00 | 17.01 |
| | ATOM | 610 | N | TRP | A | 383 | 12.261 | -7.507 | 0.294 | 1.00 | 17.61 |
| | ATOM | 611 | CA | TRP | A | 383 | 12.164 | -6.915 | -1.036 | 1.00 | 18.06 |
| 60 | ATOM | 612 | CB | TRP | A | 383 | 11.580 | -7.928 | -2.035 | 1.00 | 20.28 |
| | ATOM | 613 | CG | TRP | A | 383 | 10.105 | -8.201 | -1.919 | 1.00 | 20.50 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 614 | CD2 | TRP | A | 383 | 9.049 | -7.509 | -2.599 | 1.00 | 22.48 |
| | ATOM | 615 | CE2 | TRP | A | 383 | 7.836 | -8.138 | -2.238 | 1.00 | 20.41 |
| | ATOM | 616 | CE3 | TRP | A | 383 | 9.012 | -6.420 | -3.482 | 1.00 | 22.06 |
| | ATOM | 617 | CD1 | TRP | A | 383 | 9.506 | -9.189 | -1.190 | 1.00 | 23.38 |
| | ATOM | 618 | NE1 | TRP | A | 383 | 8.142 | -9.159 | -1.377 | 1.00 | 22.59 |
| 10 | ATOM | 619 | CZ2 | TRP | A | 383 | 6.598 | -7.713 | -2.724 | 1.00 | 21.98 |
| | ATOM | 620 | CZ3 | TRP | A | 383 | 7.780 | -5.998 | -3.968 | 1.00 | 25.50 |
| | ATOM | 621 | CH2 | TRP | A | 383 | 6.589 | -6.647 | -3.587 | 1.00 | 23.11 |
| | ATOM | 622 | C | TRP | A | 383 | 11.448 | -5.564 | -1.170 | 1.00 | 19.18 |
| | ATOM | 623 | O | TRP | A | 383 | 11.972 | -4.663 | -1.824 | 1.00 | 19.27 |
| 15 | ATOM | 624 | N | LEU | A | 384 | 10.273 | -5.396 | -0.567 | 1.00 | 18.32 |
| | ATOM | 625 | CA | LEU | A | 384 | 9.586 | -4.118 | -0.719 | 1.00 | 16.38 |
| | ATOM | 626 | CB | LEU | A | 384 | 8.125 | -4.218 | -0.258 | 1.00 | 16.79 |
| | ATOM | 627 | CG | LEU | A | 384 | 7.211 | -3.013 | -0.577 | 1.00 | 18.39 |
| | ATOM | 628 | CD1 | LEU | A | 384 | 7.464 | -2.485 | -1.995 | 1.00 | 13.91 |
| 20 | ATOM | 629 | CD2 | LEU | A | 384 | 5.750 | -3.432 | -0.410 | 1.00 | 18.38 |
| | ATOM | 630 | C | LEU | A | 384 | 10.324 | -3.027 | 0.051 | 1.00 | 18.80 |
| | ATOM | 631 | O | LEU | A | 384 | 10.334 | -1.870 | -0.357 | 1.00 | 20.90 |
| | ATOM | 632 | N | GLU | A | 385 | 10.949 | -3.404 | 1.163 | 1.00 | 18.61 |
| | ATOM | 633 | CA | GLU | A | 385 | 11.718 | -2.462 | 1.970 | 1.00 | 19.58 |
| 25 | ATOM | 634 | CB | GLU | A | 385 | 12.274 | -3.154 | 3.213 | 1.00 | 17.43 |
| | ATOM | 635 | CG | GLU | A | 385 | 11.292 | -3.237 | 4.357 | 1.00 | 22.92 |
| | ATOM | 636 | CD | GLU | A | 385 | 11.963 | -3.676 | 5.640 | 1.00 | 25.83 |
| | ATOM | 637 | OE1 | GLU | A | 385 | 12.431 | -2.799 | 6.391 | 1.00 | 23.69 |
| | ATOM | 638 | OE2 | GLU | A | 385 | 12.027 | -4.897 | 5.889 | 1.00 | 27.64 |
| 30 | ATOM | 639 | C | GLU | A | 385 | 12.890 | -1.934 | 1.156 | 1.00 | 19.46 |
| | ATOM | 640 | O | GLU | A | 385 | 13.206 | -0.743 | 1.196 | 1.00 | 15.04 |
| | ATOM | 641 | N | ILE | A | 386 | 13.539 | -2.842 | 0.431 | 1.00 | 13.32 |
| | ATOM | 642 | CA | ILE | A | 386 | 14.685 | -2.484 | -0.388 | 1.00 | 15.01 |
| | ATOM | 643 | CB | ILE | A | 386 | 15.475 | -3.763 | -0.807 | 1.00 | 17.43 |
| 35 | ATOM | 644 | CG2 | ILE | A | 386 | 16.544 | -3.424 | -1.849 | 1.00 | 17.99 |
| | ATOM | 645 | CG1 | ILE | A | 386 | 16.185 | -4.338 | 0.432 | 1.00 | 20.31 |
| | ATOM | 646 | CD1 | ILE | A | 386 | 16.682 | -5.766 | 0.284 | 1.00 | 23.97 |
| | ATOM | 647 | C | ILE | A | 386 | 14.273 | -1.645 | -1.598 | 1.00 | 16.10 |
| | ATOM | 648 | O | ILE | A | 386 | 14.993 | -0.724 | -2.004 | 1.00 | 17.42 |
| 40 | ATOM | 649 | N | LEU | A | 387 | 13.112 | -1.944 | -2.167 | 1.00 | 17.61 |
| | ATOM | 650 | CA | LEU | A | 387 | 12.620 | -1.173 | -3.304 | 1.00 | 18.20 |
| | ATOM | 651 | CB | LEU | A | 387 | 11.359 | -1.814 | -3.882 | 1.00 | 17.51 |
| | ATOM | 652 | CG | LEU | A | 387 | 11.519 | -3.064 | -4.747 | 1.00 | 26.37 |
| | ATOM | 653 | CD1 | LEU | A | 387 | 10.173 | -3.406 | -5.395 | 1.00 | 24.63 |
| 45 | ATOM | 654 | CD2 | LEU | A | 387 | 12.589 | -2.824 | -5.808 | 1.00 | 21.58 |
| | ATOM | 655 | C | LEU | A | 387 | 12.283 | 0.249 | -2.838 | 1.00 | 17.60 |
| | ATOM | 656 | O | LEU | A | 387 | 12.571 | 1.224 | -3.530 | 1.00 | 17.15 |
| | ATOM | 657 | N | MET | A | 388 | 11.677 | 0.357 | -1.660 | 1.00 | 17.65 |
| | ATOM | 658 | CA | MET | A | 388 | 11.286 | 1.656 | -1.121 | 1.00 | 18.49 |
| 50 | ATOM | 659 | CB | MET | A | 388 | 10.302 | 1.460 | 0.034 | 1.00 | 19.65 |
| | ATOM | 660 | CG | MET | A | 388 | 8.893 | 1.105 | -0.435 | 1.00 | 15.12 |
| | ATOM | 661 | SD | MET | A | 388 | 7.744 | 0.769 | 0.910 | 1.00 | 18.73 |
| | ATOM | 662 | CE | MET | A | 388 | 6.163 | 0.908 | 0.048 | 1.00 | 18.34 |
| | ATOM | 663 | C | MET | A | 388 | 12.451 | 2.553 | -0.691 | 1.00 | 22.62 |
| 55 | ATOM | 664 | O | MET | A | 388 | 12.417 | 3.767 | -0.928 | 1.00 | 22.49 |
| | ATOM | 665 | N | ILE | A | 389 | 13.482 | 1.988 | -0.064 | 1.00 | 21.45 |
| | ATOM | 666 | CA | ILE | A | 389 | 14.604 | 2.831 | 0.331 | 1.00 | 18.54 |
| | ATOM | 667 | CB | ILE | A | 389 | 15.590 | 2.108 | 1.299 | 1.00 | 19.35 |
| | ATOM | 668 | CG2 | ILE | A | 389 | 16.362 | 0.998 | 0.578 | 1.00 | 15.50 |
| 60 | ATOM | 669 | CG1 | ILE | A | 389 | 16.556 | 3.142 | 1.889 | 1.00 | 21.95 |
| | ATOM | 670 | CD1 | ILE | A | 389 | 17.373 | 2.658 | 3.080 | 1.00 | 15.86 |

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 671 | C | ILE | A | 389 | 15.333 | 3.322 | -0.922 | 1.00 | 18.67 |
| | ATOM | 672 | O | ILE | A | 389 | 15.813 | 4.453 | -0.970 | 1.00 | 19.75 |
| | ATOM | 673 | N | GLY | A | 390 | 15.410 | 2.477 | -1.943 | 1.00 | 20.58 |
| | ATOM | 674 | CA | GLY | A | 390 | 16.049 | 2.895 | -3.183 | 1.00 | 19.33 |
| | ATOM | 675 | C | GLY | A | 390 | 15.243 | 4.021 | -3.819 | 1.00 | 17.48 |
| 10 | ATOM | 676 | O | GLY | A | 390 | 15.801 | 4.994 | -4.318 | 1.00 | 21.87 |
| | ATOM | 677 | N | LEU | A | 391 | 13.920 | 3.888 | -3.787 | 1.00 | 19.17 |
| | ATOM | 678 | CA | LEU | A | 391 | 13.018 | 4.887 | -4.343 | 1.00 | 21.50 |
| | ATOM | 679 | CB | LEU | A | 391 | 11.561 | 4.420 | -4.194 | 1.00 | 18.25 |
| | ATOM | 680 | CG | LEU | A | 391 | 10.480 | 5.497 | -4.342 | 1.00 | 21.98 |
| 15 | ATOM | 681 | CD1 | LEU | A | 391 | 10.579 | 6.156 | -5.725 | 1.00 | 21.39 |
| | ATOM | 682 | CD2 | LEU | A | 391 | 9.115 | 4.868 | -4.148 | 1.00 | 17.15 |
| | ATOM | 683 | C | LEU | A | 391 | 13.208 | 6.216 | -3.620 | 1.00 | 23.27 |
| | ATOM | 684 | O | LEU | A | 391 | 13.440 | 7.255 | -4.243 | 1.00 | 23.60 |
| | ATOM | 685 | N | VAL | A | 392 | 13.122 | 6.170 | -2.295 | 1.00 | 23.04 |
| 20 | ATOM | 686 | CA | VAL | A | 392 | 13.282 | 7.357 | -1.469 | 1.00 | 24.42 |
| | ATOM | 687 | CB | VAL | A | 392 | 13.186 | 6.993 | 0.042 | 1.00 | 27.38 |
| | ATOM | 688 | CG1 | VAL | A | 392 | 13.733 | 8.129 | 0.897 | 1.00 | 30.37 |
| | ATOM | 689 | CG2 | VAL | A | 392 | 11.739 | 6.712 | 0.414 | 1.00 | 23.48 |
| | ATOM | 690 | C | VAL | A | 392 | 14.626 | 8.014 | -1.754 | 1.00 | 27.55 |
| 25 | ATOM | 691 | O | VAL | A | 392 | 14.728 | 9.242 | -1.832 | 1.00 | 27.50 |
| | ATOM | 692 | N | TRP | A | 393 | 15.652 | 7.186 | -1.924 | 1.00 | 23.65 |
| | ATOM | 693 | CA | TRP | A | 393 | 16.999 | 7.670 | -2.204 | 1.00 | 24.76 |
| | ATOM | 694 | CB | TRP | A | 393 | 17.977 | 6.491 | -2.199 | 1.00 | 22.86 |
| | ATOM | 695 | CG | TRP | A | 393 | 19.287 | 6.784 | -2.857 | 1.00 | 25.90 |
| 30 | ATOM | 696 | CD2 | TRP | A | 393 | 20.341 | 7.605 | -2.339 | 1.00 | 28.09 |
| | ATOM | 697 | CE2 | TRP | A | 393 | 21.375 | 7.612 | -3.302 | 1.00 | 29.94 |
| | ATOM | 698 | CE3 | TRP | A | 393 | 20.512 | 8.335 | -1.154 | 1.00 | 30.20 |
| | ATOM | 699 | CD1 | TRP | A | 393 | 19.710 | 6.339 | -4.077 | 1.00 | 26.55 |
| | ATOM | 700 | NE1 | TRP | A | 393 | 20.963 | 6.833 | -4.351 | 1.00 | 30.64 |
| 35 | ATOM | 701 | CZ2 | TRP | A | 393 | 22.566 | 8.323 | -3.120 | 1.00 | 32.43 |
| | ATOM | 702 | CZ3 | TRP | A | 393 | 21.698 | 9.044 | -0.971 | 1.00 | 34.58 |
| | ATOM | 703 | CH2 | TRP | A | 393 | 22.709 | 9.030 | -1.950 | 1.00 | 36.54 |
| | ATOM | 704 | C | TRP | A | 393 | 17.082 | 8.414 | -3.547 | 1.00 | 25.02 |
| | ATOM | 705 | O | TRP | A | 393 | 17.767 | 9.435 | -3.650 | 1.00 | 20.97 |
| 40 | ATOM | 706 | N | ARG | A | 394 | 16.399 | 7.897 | -4.568 | 1.00 | 23.06 |
| | ATOM | 707 | CA | ARG | A | 394 | 16.412 | 8.531 | -5.890 | 1.00 | 25.97 |
| | ATOM | 708 | CB | ARG | A | 394 | 15.776 | 7.633 | -6.965 | 1.00 | 24.05 |
| | ATOM | 709 | CG | ARG | A | 394 | 16.243 | 6.195 | -7.024 | 1.00 | 26.05 |
| | ATOM | 710 | CD | ARG | A | 394 | 15.830 | 5.551 | -8.352 | 1.00 | 22.70 |
| 45 | ATOM | 711 | NE | ARG | A | 394 | 14.443 | 5.071 | -8.363 | 1.00 | 20.71 |
| | ATOM | 712 | CZ | ARG | A | 394 | 14.053 | 3.912 | -7.841 | 1.00 | 21.26 |
| | ATOM | 713 | NH1 | ARG | A | 394 | 14.944 | 3.108 | -7.267 | 1.00 | 20.09 |
| | ATOM | 714 | NH2 | ARG | A | 394 | 12.783 | 3.544 | -7.907 | 1.00 | 21.26 |
| | ATOM | 715 | C | ARG | A | 394 | 15.622 | 9.833 | -5.879 | 1.00 | 23.40 |
| 50 | ATOM | 716 | O | ARG | A | 394 | 15.889 | 10.729 | -6.677 | 1.00 | 28.61 |
| | ATOM | 717 | N | SER | A | 395 | 14.638 | 9.924 | -4.988 | 1.00 | 26.65 |
| | ATOM | 718 | CA | SER | A | 395 | 13.776 | 11.104 | -4.902 | 1.00 | 27.46 |
| | ATOM | 719 | CB | SER | A | 395 | 12.395 | 10.696 | -4.382 | 1.00 | 26.70 |
| | ATOM | 720 | OG | SER | A | 395 | 11.916 | 9.530 | -5.029 | 1.00 | 22.95 |
| 55 | ATOM | 721 | C | SER | A | 395 | 14.316 | 12.240 | -4.033 | 1.00 | 31.45 |
| | ATOM | 722 | O | SER | A | 395 | 13.726 | 13.324 | -3.977 | 1.00 | 28.11 |
| | ATOM | 723 | N | MET | A | 396 | 15.437 | 11.986 | -3.368 | 1.00 | 33.83 |
| | ATOM | 724 | CA | MET | A | 396 | 16.061 | 12.954 | -2.475 | 1.00 | 38.83 |
| | ATOM | 725 | CB | MET | A | 396 | 17.466 | 12.483 | -2.112 | 1.00 | 39.47 |
| 60 | ATOM | 726 | CG | MET | A | 396 | 17.585 | 11.919 | -0.715 | 1.00 | 41.37 |
| | ATOM | 727 | SD | MET | A | 396 | 19.192 | 12.262 | 0.004 | 1.00 | 42.20 |

| | | | | | | | | | | | |
|----|------|-----|-----|-----|---|-----|--------|--------|---------|------|-------|
| 5 | ATOM | 728 | CE | MET | A | 396 | 20.263 | 11.996 | -1.404 | 1.00 | 42.84 |
| | ATOM | 729 | C | MET | A | 396 | 16.143 | 14.376 | -3.018 | 1.00 | 40.69 |
| | ATOM | 730 | O | MET | A | 396 | 15.637 | 15.316 | -2.403 | 1.00 | 38.85 |
| | ATOM | 731 | N | GLU | A | 397 | 16.794 | 14.526 | -4.166 | 1.00 | 42.19 |
| | ATOM | 732 | CA | GLU | A | 397 | 16.971 | 15.831 | -4.790 | 1.00 | 44.80 |
| 10 | ATOM | 733 | CB | GLU | A | 397 | 18.184 | 15.785 | -5.729 | 1.00 | 46.02 |
| | ATOM | 734 | CG | GLU | A | 397 | 17.883 | 15.189 | -7.096 | 1.00 | 54.42 |
| | ATOM | 735 | CD | GLU | A | 397 | 19.117 | 14.665 | -7.810 | 1.00 | 59.40 |
| | ATOM | 736 | OE1 | GLU | A | 397 | 19.219 | 13.430 | -7.990 | 1.00 | 60.63 |
| | ATOM | 737 | OE2 | GLU | A | 397 | 19.980 | 15.485 | -8.196 | 1.00 | 62.71 |
| 15 | ATOM | 738 | C | GLU | A | 397 | 15.735 | 16.322 | -5.554 | 1.00 | 42.94 |
| | ATOM | 739 | O | GLU | A | 397 | 15.830 | 17.229 | -6.376 | 1.00 | 44.68 |
| | ATOM | 740 | N | HIS | A | 398 | 14.579 | 15.728 | -5.280 | 1.00 | 40.82 |
| | ATOM | 741 | CA | HIS | A | 398 | 13.342 | 16.118 | -5.950 | 1.00 | 39.21 |
| | ATOM | 742 | CB | HIS | A | 398 | 12.924 | 15.043 | -6.956 | 1.00 | 39.05 |
| 20 | ATOM | 743 | CG | HIS | A | 398 | 13.870 | 14.886 | -8.104 | 1.00 | 41.57 |
| | ATOM | 744 | CD2 | HIS | A | 398 | 13.904 | 15.484 | -9.318 | 1.00 | 39.28 |
| | ATOM | 745 | ND1 | HIS | A | 398 | 14.940 | 14.017 | -8.074 | 1.00 | 41.85 |
| | ATOM | 746 | CE1 | HIS | A | 398 | 15.592 | 14.086 | -9.220 | 1.00 | 40.88 |
| | ATOM | 747 | NE2 | HIS | A | 398 | 14.985 | 14.969 | -9.993 | 1.00 | 42.30 |
| 25 | ATOM | 748 | C | HIS | A | 398 | 12.216 | 16.332 | -4.944 | 1.00 | 37.04 |
| | ATOM | 749 | O | HIS | A | 398 | 11.282 | 15.535 | -4.864 | 1.00 | 36.51 |
| | ATOM | 750 | N | PRO | A | 399 | 12.283 | 17.427 | -4.171 | 1.00 | 39.19 |
| | ATOM | 751 | CD | PRO | A | 399 | 13.328 | 18.467 | -4.198 | 1.00 | 35.36 |
| | ATOM | 752 | CA | PRO | A | 399 | 11.243 | 17.709 | -3.173 | 1.00 | 37.10 |
| 30 | ATOM | 753 | CB | PRO | A | 399 | 11.603 | 19.101 | -2.654 | 1.00 | 37.86 |
| | ATOM | 754 | CG | PRO | A | 399 | 13.050 | 19.267 | -2.963 | 1.00 | 35.83 |
| | ATOM | 755 | C | PRO | A | 399 | 9.828 | 17.663 | -3.744 | 1.00 | 37.02 |
| | ATOM | 756 | O | PRO | A | 399 | 9.554 | 18.249 | -4.789 | 1.00 | 38.52 |
| | ATOM | 757 | N | GLY | A | 400 | 8.938 | 16.954 | -3.057 | 1.00 | 33.58 |
| 35 | ATOM | 758 | CA | GLY | A | 400 | 7.559 | 16.865 | -3.503 | 1.00 | 32.12 |
| | ATOM | 759 | C | GLY | A | 400 | 7.230 | 15.706 | -4.428 | 1.00 | 32.43 |
| | ATOM | 760 | O | GLY | A | 400 | 6.063 | 15.344 | -4.574 | 1.00 | 33.21 |
| | ATOM | 761 | N | LYS | A | 401 | 8.237 | 15.112 | -5.055 | 1.00 | 31.35 |
| | ATOM | 762 | CA | LYS | A | 401 | 7.972 | 14.007 | -5.966 | 1.00 | 30.75 |
| 40 | ATOM | 763 | CB | LYS | A | 401 | 8.235 | 14.430 | -7.415 | 1.00 | 35.43 |
| | ATOM | 764 | CG | LYS | A | 401 | 8.130 | 15.927 | -7.675 | 1.00 | 35.15 |
| | ATOM | 765 | CD | LYS | A | 401 | 9.096 | 16.353 | -8.774 | 1.00 | 36.88 |
| | ATOM | 766 | CE | LYS | A | 401 | 8.733 | 17.721 | -9.331 | 1.00 | 36.71 |
| | ATOM | 767 | NZ | LYS | A | 401 | 7.295 | 18.027 | -9.116 | 1.00 | 34.22 |
| 45 | ATOM | 768 | C | LYS | A | 401 | 8.768 | 12.746 | -5.677 | 1.00 | 30.97 |
| | ATOM | 769 | O | LYS | A | 401 | 9.809 | 12.776 | -5.006 | 1.00 | 27.60 |
| | ATOM | 770 | N | LEU | A | 402 | 8.256 | 11.635 | -6.197 | 1.00 | 27.28 |
| | ATOM | 771 | CA | LEU | A | 402 | 8.889 | 10.334 | -6.050 | 1.00 | 29.07 |
| | ATOM | 772 | CB | LEU | A | 402 | 7.866 | 9.294 | -5.590 | 1.00 | 22.55 |
| 50 | ATOM | 773 | CG | LEU | A | 402 | 7.265 | 9.555 | -4.207 | 1.00 | 24.94 |
| | ATOM | 774 | CD1 | LEU | A | 402 | 6.126 | 8.583 | -3.937 | 1.00 | 19.32 |
| | ATOM | 775 | CD2 | LEU | A | 402 | 8.355 | 9.416 | -3.157 | 1.00 | 21.54 |
| | ATOM | 776 | C | LEU | A | 402 | 9.448 | 9.948 | -7.414 | 1.00 | 28.78 |
| | ATOM | 777 | O | LEU | A | 402 | 8.704 | 9.836 | -8.389 | 1.00 | 29.98 |
| 55 | ATOM | 778 | N | LEU | A | 403 | 10.761 | 9.770 | -7.487 | 1.00 | 27.57 |
| | ATOM | 779 | CA | LEU | A | 403 | 11.393 | 9.400 | -8.744 | 1.00 | 27.17 |
| | ATOM | 780 | CB | LEU | A | 403 | 12.825 | 9.937 | -8.816 | 1.00 | 26.95 |
| | ATOM | 781 | CG | LEU | A | 403 | 13.401 | 10.027 | -10.238 | 1.00 | 30.42 |
| | ATOM | 782 | CD1 | LEU | A | 403 | 14.519 | 11.046 | -10.288 | 1.00 | 30.76 |
| 60 | ATOM | 783 | CD2 | LEU | A | 403 | 13.915 | 8.665 | -10.676 | 1.00 | 33.11 |
| | ATOM | 784 | C | LEU | A | 403 | 11.419 | 7.891 | -8.901 | 1.00 | 24.78 |

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|----|------|-----|-----|-----|---|-----|--------|--------|---------|------|-------|
| 5 | ATOM | 785 | O | LEU | A | 403 | 12.428 | 7.257 | -8.619 | 1.00 | 24.68 |
| | ATOM | 786 | N | PHE | A | 404 | 10.306 | 7.319 | -9.344 | 1.00 | 23.11 |
| | ATOM | 787 | CA | PHE | A | 404 | 10.239 | 5.881 | -9.546 | 1.00 | 26.93 |
| | ATOM | 788 | CB | PHE | A | 404 | 8.826 | 5.470 | -9.946 | 1.00 | 27.04 |
| | ATOM | 789 | CG | PHE | A | 404 | 7.850 | 5.513 | -8.816 | 1.00 | 27.89 |
| 10 | ATOM | 790 | CD1 | PHE | A | 404 | 7.028 | 6.623 | -8.631 | 1.00 | 26.20 |
| | ATOM | 791 | CD2 | PHE | A | 404 | 7.750 | 4.444 | -7.925 | 1.00 | 23.10 |
| | ATOM | 792 | CE1 | PHE | A | 404 | 6.116 | 6.668 | -7.573 | 1.00 | 25.29 |
| | ATOM | 793 | CE2 | PHE | A | 404 | 6.845 | 4.481 | -6.870 | 1.00 | 21.01 |
| | ATOM | 794 | CZ | PHE | A | 404 | 6.026 | 5.595 | -6.693 | 1.00 | 22.91 |
| 15 | ATOM | 795 | C | PHE | A | 404 | 11.232 | 5.507 | -10.637 | 1.00 | 26.04 |
| | ATOM | 796 | O | PHE | A | 404 | 11.882 | 4.464 | -10.578 | 1.00 | 27.27 |
| | ATOM | 797 | N | ALA | A | 405 | 11.348 | 6.383 | -11.626 | 1.00 | 28.80 |
| | ATOM | 798 | CA | ALA | A | 405 | 12.271 | 6.195 | -12.740 | 1.00 | 29.21 |
| | ATOM | 799 | CB | ALA | A | 405 | 11.650 | 5.287 | -13.806 | 1.00 | 26.89 |
| 20 | ATOM | 800 | C | ALA | A | 405 | 12.549 | 7.578 | -13.317 | 1.00 | 30.23 |
| | ATOM | 801 | O | ALA | A | 405 | 11.770 | 8.508 | -13.109 | 1.00 | 27.38 |
| | ATOM | 802 | N | PRO | A | 406 | 13.672 | 7.737 | -14.032 | 1.00 | 30.05 |
| | ATOM | 803 | CD | PRO | A | 406 | 14.712 | 6.745 | -14.352 | 1.00 | 26.31 |
| | ATOM | 804 | CA | PRO | A | 406 | 13.977 | 9.053 | -14.604 | 1.00 | 32.10 |
| 25 | ATOM | 805 | CB | PRO | A | 406 | 15.232 | 8.800 | -15.438 | 1.00 | 31.28 |
| | ATOM | 806 | CG | PRO | A | 406 | 15.865 | 7.602 | -14.776 | 1.00 | 31.44 |
| | ATOM | 807 | C | PRO | A | 406 | 12.820 | 9.589 | -15.436 | 1.00 | 32.58 |
| | ATOM | 808 | O | PRO | A | 406 | 12.605 | 10.796 | -15.507 | 1.00 | 32.58 |
| | ATOM | 809 | N | ASN | A | 407 | 12.063 | 8.690 | -16.053 | 1.00 | 32.86 |
| 30 | ATOM | 810 | CA | ASN | A | 407 | 10.935 | 9.119 | -16.865 | 1.00 | 32.78 |
| | ATOM | 811 | CB | ASN | A | 407 | 10.950 | 8.418 | -18.228 | 1.00 | 34.73 |
| | ATOM | 812 | CG | ASN | A | 407 | 10.884 | 6.907 | -18.121 | 1.00 | 35.37 |
| | ATOM | 813 | OD1 | ASN | A | 407 | 11.189 | 6.317 | -17.077 | 1.00 | 30.24 |
| | ATOM | 814 | ND2 | ASN | A | 407 | 10.486 | 6.268 | -19.215 | 1.00 | 34.08 |
| 35 | ATOM | 815 | C | ASN | A | 407 | 9.605 | 8.901 | -16.166 | 1.00 | 34.90 |
| | ATOM | 816 | O | ASN | A | 407 | 8.549 | 8.897 | -16.798 | 1.00 | 36.09 |
| | ATOM | 817 | N | LEU | A | 408 | 9.660 | 8.724 | -14.851 | 1.00 | 33.56 |
| | ATOM | 818 | CA | LEU | A | 408 | 8.452 | 8.544 | -14.061 | 1.00 | 35.59 |
| | ATOM | 819 | CB | LEU | A | 408 | 8.141 | 7.062 | -13.851 | 1.00 | 33.81 |
| 40 | ATOM | 820 | CG | LEU | A | 408 | 6.696 | 6.823 | -13.397 | 1.00 | 36.44 |
| | ATOM | 821 | CD1 | LEU | A | 408 | 5.746 | 7.479 | -14.390 | 1.00 | 34.14 |
| | ATOM | 822 | CD2 | LEU | A | 408 | 6.406 | 5.334 | -13.287 | 1.00 | 32.96 |
| | ATOM | 823 | C | LEU | A | 408 | 8.607 | 9.245 | -12.717 | 1.00 | 38.03 |
| | ATOM | 824 | O | LEU | A | 408 | 8.880 | 8.614 | -11.695 | 1.00 | 36.38 |
| 45 | ATOM | 825 | N | LEU | A | 409 | 8.441 | 10.563 | -12.741 | 1.00 | 37.87 |
| | ATOM | 826 | CA | LEU | A | 409 | 8.548 | 11.395 | -11.553 | 1.00 | 37.95 |
| | ATOM | 827 | CB | LEU | A | 409 | 9.373 | 12.636 | -11.877 | 1.00 | 39.52 |
| | ATOM | 828 | CG | LEU | A | 409 | 10.023 | 13.399 | -10.728 | 1.00 | 42.46 |
| | ATOM | 829 | CD1 | LEU | A | 409 | 11.100 | 12.547 | -10.082 | 1.00 | 43.24 |
| 50 | ATOM | 830 | CD2 | LEU | A | 409 | 10.614 | 14.691 | -11.266 | 1.00 | 46.05 |
| | ATOM | 831 | C | LEU | A | 409 | 7.132 | 11.792 | -11.163 | 1.00 | 37.13 |
| | ATOM | 832 | O | LEU | A | 409 | 6.482 | 12.546 | -11.882 | 1.00 | 35.70 |
| | ATOM | 833 | N | LEU | A | 410 | 6.654 | 11.284 | -10.030 | 1.00 | 35.29 |
| | ATOM | 834 | CA | LEU | A | 410 | 5.297 | 11.576 | -9.583 | 1.00 | 33.33 |
| 55 | ATOM | 835 | CB | LEU | A | 410 | 4.503 | 10.277 | -9.449 | 1.00 | 29.37 |
| | ATOM | 836 | CG | LEU | A | 410 | 4.645 | 9.238 | -10.560 | 1.00 | 32.75 |
| | ATOM | 837 | CD1 | LEU | A | 410 | 4.026 | 7.925 | -10.104 | 1.00 | 29.16 |
| | ATOM | 838 | CD2 | LEU | A | 410 | 3.958 | 9.744 | -11.819 | 1.00 | 30.70 |
| | ATOM | 839 | C | LEU | A | 410 | 5.207 | 12.332 | -8.261 | 1.00 | 35.14 |
| 60 | ATOM | 840 | O | LEU | A | 410 | 6.078 | 12.214 | -7.400 | 1.00 | 36.94 |
| | ATOM | 841 | N | ASP | A | 411 | 4.141 | 13.108 | -8.105 | 1.00 | 34.76 |

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|----|------|-----|-----|-----|---|-----|--------|-------------------|-------------------|------|-------|
| 5 | ATOM | 842 | CA | ASP | A | 411 | 3.933 | 13.843 | -6.873 | 1.00 | 35.40 |
| | ATOM | 843 | CB | ASP | A | 411 | 3.733 | 15.341 | -7.144 | 1.00 | 40.02 |
| | ATOM | 844 | CG | ASP | A | 411 | 2.471 | 15.645 | -7.928 | 1.00 | 41.32 |
| | ATOM | 845 | OD1 | ASP | A | 411 | 1.570 | 14.785 | -8.001 | 1.00 | 45.03 |
| | ATOM | 846 | OD2 | ASP | A | 411 | 2.383 | 16.764 | -8.474 | 1.00 | 45.01 |
| 10 | ATOM | 847 | C | ASP | A | 411 | 2.727 | 13.234 | -6.179 | 1.00 | 36.10 |
| | ATOM | 848 | O | ASP | A | 411 | 2.033 | 12.395 | -6.762 | 1.00 | 34.08 |
| | ATOM | 849 | N | ARG | A | 412 | 2.480 | 13.647 | -4.940 | 1.00 | 35.99 |
| | ATOM | 850 | CA | ARG | A | 412 | 1.375 | 13.099 | -4.169 | 1.00 | 39.37 |
| | ATOM | 851 | CB | ARG | A | 412 | 1.260 | 13.824 | -2.825 | 1.00 | 39.75 |
| 15 | ATOM | 852 | CG | ARG | A | 412 | 0.562 | 15.168 | -2.870 | 1.00 | 40.49 |
| | ATOM | 853 | CD | ARG | A | 412 | 0.454 | 15.736 | -1.465 | 1.00 | 40.65 |
| | ATOM | 854 | NE | ARG | A | 412 | -0.261 | 14.826 | -0.577 | 1.00 | 37.48 |
| | ATOM | 855 | CZ | ARG | A | 412 | -1.574 | 14.855 | -0.384 | 1.00 | 42.84 |
| | ATOM | 856 | NH1 | ARG | A | 412 | -2.316 | 15.754 | -1.024 | 1.00 | 40.82 |
| 20 | ATOM | 857 | NH2 | ARG | A | 412 | -2.150 | 13.986 | 0.438 | 1.00 | 38.32 |
| | ATOM | 858 | C | ARG | A | 412 | 0.034 | 13.108 | -4.889 | 1.00 | 39.80 |
| | ATOM | 859 | O | ARG | A | 412 | -0.775 | 12.201 | -4.706 | 1.00 | 39.92 |
| | ATOM | 860 | N | ASN | A | 413 | -0.198 | 14.119 | -5.717 | 1.00 | 41.64 |
| | ATOM | 861 | CA | ASN | A | 413 | -1.458 | 14.215 | -6.440 | 1.00 | 43.19 |
| 25 | ATOM | 862 | CB | ASN | A | 413 | -1.518 | 15.533 | -7.210 | 1.00 | 46.44 |
| | ATOM | 863 | CG | ASN | A | 413 | -1.739 | 16.718 | -6.299 | 1.00 | 47.86 |
| | ATOM | 864 | OD1 | ASN | A | 413 | -2.376 | 16.594 | -5.249 | 1.00 | 48.05 |
| | ATOM | 865 | ND2 | ASN | A | 413 | -1.213 | 17.876 | -6.687 | 1.00 | 49.43 |
| | ATOM | 866 | C | ASN | A | 413 | -1.673 | 13.044 | -7.385 | 1.00 | 41.48 |
| 30 | ATOM | 867 | O | ASN | A | 413 | -2.792 | 12.567 | -7.546 | 1.00 | 40.50 |
| | ATOM | 868 | N | GLN | A | 414 | -0.600 | 12.577 | -8.010 | 1.00 | 42.82 |
| | ATOM | 869 | CA | GLN | A | 414 | -0.703 | 11.448 | -8.925 | 1.00 | 44.73 |
| | ATOM | 870 | CB | GLN | A | 414 | 0.585 | 11.307 | -9.741 | 1.00 | 47.52 |
| | ATOM | 871 | CG | GLN | A | 414 | 0.572 | 12.088 | -11.049 | 1.00 | 50.47 |
| 35 | ATOM | 872 | CD | GLN | A | 414 | 1.914 | 12.713 | -11.375 | 1.00 | 53.91 |
| | ATOM | 873 | OE1 | GLN | A | 414 | 2.591 | 13.257 | -10.501 | 1.00 | 53.68 |
| | ATOM | 874 | NE2 | GLN | A | 414 | 2.309 | 12.637 | -12.641 | 1.00 | 56.91 |
| | ATOM | 875 | C | GLN | A | 414 | -0.970 | 10.163 | -8.141 | 1.00 | 43.21 |
| | ATOM | 876 | O | GLN | A | 414 | -1.491 | 9.193 | -8.682 | 1.00 | 42.33 |
| 40 | ATOM | 877 | N | GLY | A | 415 | -0.618 | 10.168 | -6.860 | 1.00 | 41.97 |
| | ATOM | 878 | CA | GLY | A | 415 | -0.836 | 8.992 | -6.040 | 1.00 | 40.43 |
| | ATOM | 879 | C | GLY | A | 415 | -2.306 | 8.720 | -5.804 | 1.00 | 40.80 |
| | ATOM | 880 | O | GLY | A | 415 | -2.696 | 7.601 | -5.472 | 1.00 | 37.83 |
| | ATOM | 881 | N | LYS | A | 416 | -3.129 | 9.748 | -5.978 | 1.00 | 42.16 |
| 45 | ATOM | 882 | CA | LYS | A | 416 | -4.566 | 9.613 | -5.779 | 1.00 | 44.34 |
| | ATOM | 883 | CB | LYS | A | 416 | -5.212 | 10.996 | -5.704 | 1.00 | 45.65 |
| | ATOM | 884 | CG | LYS | A | 416 | -4.761 | 11.819 | -4.510 | 1.00 | 47.42 |
| | ATOM | 885 | CD | LYS | A | 416 | -4.910 | 13.309 | -4.777 | 1.00 | 50.97 |
| | ATOM | 886 | CE | LYS | A | 416 | -5.992 | 13.924 | -3.898 | 1.00 | 53.25 |
| 50 | ATOM | 887 | NZ | LYS | A | 416 | -5.416 | 14.764 | -2.809 | 1.00 | 56.95 |
| | ATOM | 888 | C | LYS | A | 416 | -5.227 | 8.793 | -6.886 | 1.00 | 45.33 |
| | ATOM | 889 | O | LYS | A | 416 | -6.339 | 8.299 | -6.714 | 1.00 | 46.50 |
| | ATOM | 890 | N | CYS | A | 417 | -4.540 | 8.648 | -8.015 | 1.00 | 45.18 |
| | ATOM | 891 | CA | CYS | A | 417 | -5.066 | 7.890 | -9.148 | 1.00 | 46.25 |
| 55 | ATOM | 892 | CB | CYS | A | 417 | -4.062 | 7.902 | -10.305 | 1.00 | 49.29 |
| | ATOM | 893 | SG | CYS | A | 417 | -3.916 | 9.493 | -11.168 | 1.00 | 49.59 |
| | ATOM | 894 | C | CYS | A | 417 | -5.373 | 6.452 | -8.752 | 1.00 | 47.18 |
| | ATOM | 895 | O | CYS | A | 417 | -6.220 | 5.794 | -9.359 | 1.00 | 46.50 |
| | ATOM | 896 | N | VAL | A | 418 | -4.671 | 5.968 | -7.731 | 1.00 | 45.07 |
| 60 | ATOM | 897 | CA | VAL | A | 418 | -4.866 | 4.612 | -7.232 | 1.00 | 42.75 |
| | ATOM | 898 | CB | VAL | A | 418 | -3.525 | 3.841 | -7.206 | 1.00 | 42.45 |

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|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|
| 5 | ATOM | 899 | CG1 | VAL | A | 418 | -3.670 | 2.563 | -6.410 | 1.00 | 40.22 |
| | ATOM | 900 | CG2 | VAL | A | 418 | -3.071 | 3.538 | -8.634 | 1.00 | 38.03 |
| | ATOM | 901 | C | VAL | A | 418 | -5.441 | 4.714 | -5.818 | 1.00 | 41.46 |
| | ATOM | 902 | O | VAL | A | 418 | -4.883 | 5.400 | -4.963 | 1.00 | 42.08 |
| | ATOM | 903 | N | GLU | A | 419 | -6.559 | 4.036 | -5.579 | 1.00 | 40.95 |
| 10 | ATOM | 904 | CA | GLU | A | 419 | -7.223 | 4.073 | -4.275 | 1.00 | 42.51 |
| | ATOM | 905 | CB | GLU | A | 419 | -8.536 | 3.282 | -4.333 | 1.00 | 44.52 |
| | ATOM | 906 | CG | GLU | A | 419 | -9.010 | 2.751 | -2.984 | 1.00 | 50.42 |
| | ATOM | 907 | CD | GLU | A | 419 | -10.413 | 2.168 | -3.035 | 1.00 | 54.38 |
| | ATOM | 908 | OE1 | GLU | A | 419 | -10.582 | 1.059 | -3.590 | 1.00 | 54.09 |
| 15 | ATOM | 909 | OE2 | GLU | A | 419 | -11.347 | 2.820 | -2.516 | 1.00 | 57.90 |
| | ATOM | 910 | C | GLU | A | 419 | -6.370 | 3.552 | -3.121 | 1.00 | 41.11 |
| | ATOM | 911 | O | GLU | A | 419 | -5.955 | 2.393 | -3.116 | 1.00 | 39.42 |
| | ATOM | 912 | N | GLY | A | 420 | -6.129 | 4.419 | -2.140 | 1.00 | 40.53 |
| | ATOM | 913 | CA | GLY | A | 420 | -5.346 | 4.049 | -0.973 | 1.00 | 37.61 |
| 20 | ATOM | 914 | C | GLY | A | 420 | -3.854 | 4.258 | -1.140 | 1.00 | 37.01 |
| | ATOM | 915 | O | GLY | A | 420 | -3.088 | 4.105 | -0.190 | 1.00 | 32.59 |
| | ATOM | 916 | N | MET | A | 421 | -3.444 | 4.623 | -2.350 | 1.00 | 36.21 |
| | ATOM | 917 | CA | MET | A | 421 | -2.035 | 4.825 | -2.656 | 1.00 | 36.02 |
| | ATOM | 918 | CB | MET | A | 421 | -1.799 | 4.607 | -4.160 | 1.00 | 32.84 |
| 25 | ATOM | 919 | CG | MET | A | 421 | -0.351 | 4.754 | -4.617 | 1.00 | 35.82 |
| | ATOM | 920 | SD | MET | A | 421 | 0.806 | 3.611 | -3.812 | 1.00 | 35.57 |
| | ATOM | 921 | CE | MET | A | 421 | 0.881 | 2.294 | -5.005 | 1.00 | 32.51 |
| | ATOM | 922 | C | MET | A | 421 | -1.474 | 6.180 | -2.226 | 1.00 | 34.93 |
| | ATOM | 923 | O | MET | A | 421 | -0.275 | 6.294 | -1.985 | 1.00 | 35.17 |
| 30 | ATOM | 924 | N | VAL | A | 422 | -2.319 | 7.205 | -2.118 | 1.00 | 33.97 |
| | ATOM | 925 | CA | VAL | A | 422 | -1.823 | 8.520 | -1.708 | 1.00 | 31.29 |
| | ATOM | 926 | CB | VAL | A | 422 | -2.927 | 9.607 | -1.766 | 1.00 | 33.14 |
| | ATOM | 927 | CG1 | VAL | A | 422 | -3.823 | 9.535 | -0.533 | 1.00 | 30.10 |
| | ATOM | 928 | CG2 | VAL | A | 422 | -2.279 | 10.982 | -1.854 | 1.00 | 30.08 |
| 35 | ATOM | 929 | C | VAL | A | 422 | -1.231 | 8.498 | -0.296 | 1.00 | 32.64 |
| | ATOM | 930 | O | VAL | A | 422 | -0.274 | 9.220 | 0.002 | 1.00 | 28.41 |
| | ATOM | 931 | N | GLU | A | 423 | -1.803 | 7.670 | 0.571 | 1.00 | 31.53 |
| | ATOM | 932 | CA | GLU | A | 423 | -1.311 | 7.558 | 1.935 | 1.00 | 35.99 |
| | ATOM | 933 | CB | GLU | A | 423 | -2.190 | 6.594 | 2.737 | 1.00 | 40.37 |
| 40 | ATOM | 934 | CG | GLU | A | 423 | -3.588 | 7.129 | 3.043 | 1.00 | 49.41 |
| | ATOM | 935 | CD | GLU | A | 423 | -4.438 | 7.336 | 1.795 | 1.00 | 52.38 |
| | ATOM | 936 | OE1 | GLU | A | 423 | -5.349 | 8.188 | 1.835 | 1.00 | 56.91 |
| | ATOM | 937 | OE2 | GLU | A | 423 | -4.200 | 6.652 | 0.776 | 1.00 | 54.53 |
| | ATOM | 938 | C | GLU | A | 423 | 0.127 | 7.043 | 1.886 | 1.00 | 34.83 |
| 45 | ATOM | 939 | O | GLU | A | 423 | 1.007 | 7.552 | 2.581 | 1.00 | 31.85 |
| | ATOM | 940 | N | ILE | A | 424 | 0.369 | 6.038 | 1.050 | 1.00 | 30.17 |
| | ATOM | 941 | CA | ILE | A | 424 | 1.711 | 5.488 | 0.929 | 1.00 | 28.99 |
| | ATOM | 942 | CB | ILE | A | 424 | 1.696 | 4.195 | 0.109 | 1.00 | 30.96 |
| | ATOM | 943 | CG2 | ILE | A | 424 | 3.108 | 3.588 | 0.068 | 1.00 | 27.20 |
| 50 | ATOM | 944 | CG1 | ILE | A | 424 | 0.671 | 3.230 | 0.725 | 1.00 | 30.77 |
| | ATOM | 945 | CD1 | ILE | A | 424 | 0.810 | 1.787 | 0.291 | 1.00 | 34.69 |
| | ATOM | 946 | C | ILE | A | 424 | 2.700 | 6.483 | 0.312 | 1.00 | 28.21 |
| | ATOM | 947 | O | ILE | A | 424 | 3.856 | 6.551 | 0.735 | 1.00 | 28.48 |
| | ATOM | 948 | N | PHE | A | 425 | 2.253 | 7.260 | -0.675 | 1.00 | 27.68 |
| 55 | ATOM | 949 | CA | PHE | A | 425 | 3.119 | 8.253 | -1.315 | 1.00 | 27.30 |
| | ATOM | 950 | CB | PHE | A | 425 | 2.381 | 8.958 | -2.458 | 1.00 | 26.36 |
| | ATOM | 951 | CG | PHE | A | 425 | 2.538 | 8.289 | -3.798 | 1.00 | 27.22 |
| | ATOM | 952 | CD1 | PHE | A | 425 | 2.619 | 9.050 | -4.958 | 1.00 | 27.36 |
| | ATOM | 953 | CD2 | PHE | A | 425 | 2.566 | 6.900 | -3.905 | 1.00 | 27.89 |
| 60 | ATOM | 954 | CE1 | PHE | A | 425 | 2.721 | 8.443 | -6.207 | 1.00 | 29.63 |
| | ATOM | 955 | CE2 | PHE | A | 425 | 2.668 | 6.282 | -5.149 | 1.00 | 27.28 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 956 | CZ | PHE | A | 425 | 2.745 | 9.306 | -0.312 | 1.00 | 27.63 |
| | ATOM | 957 | C | PHE | A | 425 | 3.591 | 9.306 | -0.312 | 1.00 | 25.66 |
| | ATOM | 958 | O | PHE | A | 425 | 4.757 | 9.713 | -0.328 | 1.00 | 26.33 |
| | ATOM | 959 | N | ASP | A | 426 | 2.680 | 9.746 | 0.552 | 1.00 | 27.92 |
| | ATOM | 960 | CA | ASP | A | 426 | 2.984 | 10.759 | 1.570 | 1.00 | 28.88 |
| 10 | ATOM | 961 | CB | ASP | A | 426 | 1.721 | 11.102 | 2.369 | 1.00 | 32.58 |
| | ATOM | 962 | CG | ASP | A | 426 | 0.781 | 12.034 | 1.613 | 1.00 | 37.47 |
| | ATOM | 963 | OD1 | ASP | A | 426 | -0.432 | 12.039 | 1.925 | 1.00 | 37.72 |
| | ATOM | 964 | OD2 | ASP | A | 426 | 1.253 | 12.758 | 0.710 | 1.00 | 36.35 |
| | ATOM | 965 | C | ASP | A | 426 | 4.071 | 10.278 | 2.532 | 1.00 | 26.96 |
| 15 | ATOM | 966 | O | ASP | A | 426 | 4.974 | 11.030 | 2.900 | 1.00 | 27.20 |
| | ATOM | 967 | N | MET | A | 427 | 3.978 | 9.022 | 2.947 | 1.00 | 25.76 |
| | ATOM | 968 | CA | MET | A | 427 | 4.981 | 8.468 | 3.856 | 1.00 | 25.89 |
| | ATOM | 969 | CB | MET | A | 427 | 4.567 | 7.070 | 4.309 | 1.00 | 21.17 |
| | ATOM | 970 | CG | MET | A | 427 | 3.385 | 7.072 | 5.257 | 1.00 | 24.38 |
| 20 | ATOM | 971 | SD | MET | A | 427 | 3.153 | 5.489 | 6.080 | 1.00 | 34.32 |
| | ATOM | 972 | CE | MET | A | 427 | 2.173 | 4.637 | 4.910 | 1.00 | 21.03 |
| | ATOM | 973 | C | MET | A | 427 | 6.321 | 8.410 | 3.128 | 1.00 | 22.29 |
| | ATOM | 974 | O | MET | A | 427 | 7.363 | 8.760 | 3.689 | 1.00 | 22.19 |
| | ATOM | 975 | N | LEU | A | 428 | 6.285 | 7.985 | 1.868 | 1.00 | 21.75 |
| 25 | ATOM | 976 | CA | LEU | A | 428 | 7.506 | 7.892 | 1.075 | 1.00 | 22.91 |
| | ATOM | 977 | CB | LEU | A | 428 | 7.202 | 7.252 | -0.287 | 1.00 | 18.47 |
| | ATOM | 978 | CG | LEU | A | 428 | 6.910 | 5.747 | -0.176 | 1.00 | 19.24 |
| | ATOM | 979 | CD1 | LEU | A | 428 | 6.278 | 5.222 | -1.468 | 1.00 | 16.82 |
| | ATOM | 980 | CD2 | LEU | A | 428 | 8.204 | 5.010 | 0.131 | 1.00 | 16.23 |
| 30 | ATOM | 981 | C | LEU | A | 428 | 8.148 | 9.269 | 0.902 | 1.00 | 23.98 |
| | ATOM | 982 | O | LEU | A | 428 | 9.366 | 9.416 | 1.034 | 1.00 | 23.06 |
| | ATOM | 983 | N | LEU | A | 429 | 7.328 | 10.281 | 0.628 | 1.00 | 23.91 |
| | ATOM | 984 | CA | LEU | A | 429 | 7.837 | 11.642 | 0.462 | 1.00 | 26.29 |
| | ATOM | 985 | CB | LEU | A | 429 | 6.714 | 12.571 | -0.003 | 1.00 | 27.47 |
| 35 | ATOM | 986 | CG | LEU | A | 429 | 6.331 | 12.411 | -1.476 | 1.00 | 30.78 |
| | ATOM | 987 | CD1 | LEU | A | 429 | 5.022 | 13.139 | -1.751 | 1.00 | 34.75 |
| | ATOM | 988 | CD2 | LEU | A | 429 | 7.449 | 12.952 | -2.350 | 1.00 | 31.96 |
| | ATOM | 989 | C | LEU | A | 429 | 8.425 | 12.166 | 1.776 | 1.00 | 25.83 |
| | ATOM | 990 | O | LEU | A | 429 | 9.482 | 12.808 | 1.793 | 1.00 | 26.42 |
| 40 | ATOM | 991 | N | ALA | A | 430 | 7.734 | 11.890 | 2.877 | 1.00 | 26.45 |
| | ATOM | 992 | CA | ALA | A | 430 | 8.201 | 12.333 | 4.185 | 1.00 | 26.11 |
| | ATOM | 993 | CB | ALA | A | 430 | 7.214 | 11.909 | 5.265 | 1.00 | 23.13 |
| | ATOM | 994 | C | ALA | A | 430 | 9.577 | 11.742 | 4.462 | 1.00 | 25.01 |
| | ATOM | 995 | O | ALA | A | 430 | 10.455 | 12.409 | 5.005 | 1.00 | 24.31 |
| 45 | ATOM | 996 | N | THR | A | 431 | 9.767 | 10.486 | 4.074 | 1.00 | 25.25 |
| | ATOM | 997 | CA | THR | A | 431 | 11.046 | 9.825 | 4.294 | 1.00 | 22.78 |
| | ATOM | 998 | CB | THR | A | 431 | 10.973 | 8.323 | 3.962 | 1.00 | 21.36 |
| | ATOM | 999 | OG1 | THR | A | 431 | 9.924 | 7.727 | 4.727 | 1.00 | 20.27 |
| | ATOM | 1000 | CG2 | THR | A | 431 | 12.291 | 7.633 | 4.299 | 1.00 | 19.99 |
| 50 | ATOM | 1001 | C | THR | A | 431 | 12.103 | 10.477 | 3.429 | 1.00 | 23.73 |
| | ATOM | 1002 | O | THR | A | 431 | 13.234 | 10.667 | 3.868 | 1.00 | 19.60 |
| | ATOM | 1003 | N | SER | A | 432 | 11.736 | 10.819 | 2.197 | 1.00 | 24.32 |
| | ATOM | 1004 | CA | SER | A | 432 | 12.676 | 11.479 | 1.301 | 1.00 | 26.96 |
| | ATOM | 1005 | CB | SER | A | 432 | 12.067 | 11.650 | -0.093 | 1.00 | 28.70 |
| 55 | ATOM | 1006 | OG | SER | A | 432 | 13.084 | 11.930 | -1.039 | 1.00 | 33.42 |
| | ATOM | 1007 | C | SER | A | 432 | 13.033 | 12.850 | 1.876 | 1.00 | 27.92 |
| | ATOM | 1008 | O | SER | A | 432 | 14.176 | 13.294 | 1.779 | 1.00 | 30.78 |
| | ATOM | 1009 | N | SER | A | 433 | 12.045 | 13.521 | 2.459 | 1.00 | 28.96 |
| | ATOM | 1010 | CA | SER | A | 433 | 12.269 | 14.824 | 3.076 | 1.00 | 34.21 |
| 60 | ATOM | 1011 | CB | SER | A | 433 | 10.957 | 15.387 | 3.623 | 1.00 | 35.07 |
| | ATOM | 1012 | OG | SER | A | 433 | 10.175 | 15.961 | 2.591 | 1.00 | 42.38 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1013 | C | SER | A | 433 | 13.263 | 14.644 | 4.223 | 1.00 | 33.43 |
| | ATOM | 1014 | O | SER | A | 433 | 14.152 | 15.473 | 4.429 | 1.00 | 31.94 |
| | ATOM | 1015 | N | ARG | A | 434 | 13.105 | 13.545 | 4.959 | 1.00 | 31.32 |
| | ATOM | 1016 | CA | ARG | A | 434 | 13.980 | 13.236 | 6.086 | 1.00 | 29.78 |
| | ATOM | 1017 | CB | ARG | A | 434 | 13.468 | 11.994 | 6.819 | 1.00 | 29.84 |
| 10 | ATOM | 1018 | CG | ARG | A | 434 | 14.331 | 11.541 | 7.983 | 1.00 | 32.17 |
| | ATOM | 1019 | CD | ARG | A | 434 | 14.626 | 12.672 | 8.958 | 1.00 | 37.00 |
| | ATOM | 1020 | NE | ARG | A | 434 | 15.321 | 12.169 | 10.140 | 1.00 | 39.44 |
| | ATOM | 1021 | CZ | ARG | A | 434 | 15.935 | 12.935 | 11.034 | 1.00 | 44.06 |
| | ATOM | 1022 | NH1 | ARG | A | 434 | 15.949 | 14.255 | 10.885 | 1.00 | 45.52 |
| 15 | ATOM | 1023 | NH2 | ARG | A | 434 | 16.528 | 12.381 | 12.084 | 1.00 | 45.01 |
| | ATOM | 1024 | C | ARG | A | 434 | 15.413 | 13.014 | 5.605 | 1.00 | 29.24 |
| | ATOM | 1025 | O | ARG | A | 434 | 16.352 | 13.563 | 6.173 | 1.00 | 29.72 |
| | ATOM | 1026 | N | PHE | A | 435 | 15.577 | 12.206 | 4.561 | 1.00 | 28.95 |
| | ATOM | 1027 | CA | PHE | A | 435 | 16.901 | 11.935 | 4.000 | 1.00 | 30.59 |
| 20 | ATOM | 1028 | CB | PHE | A | 435 | 16.777 | 11.045 | 2.758 | 1.00 | 32.03 |
| | ATOM | 1029 | CG | PHE | A | 435 | 16.795 | 9.563 | 3.051 | 1.00 | 31.88 |
| | ATOM | 1030 | CD1 | PHE | A | 435 | 16.758 | 9.084 | 4.359 | 1.00 | 35.60 |
| | ATOM | 1031 | CD2 | PHE | A | 435 | 16.847 | 8.643 | 2.009 | 1.00 | 35.89 |
| | ATOM | 1032 | CE1 | PHE | A | 435 | 16.771 | 7.709 | 4.622 | 1.00 | 35.36 |
| 25 | ATOM | 1033 | CE2 | PHE | A | 435 | 16.860 | 7.271 | 2.262 | 1.00 | 32.71 |
| | ATOM | 1034 | CZ | PHE | A | 435 | 16.821 | 6.807 | 3.570 | 1.00 | 33.24 |
| | ATOM | 1035 | C | PHE | A | 435 | 17.576 | 13.253 | 3.607 | 1.00 | 32.73 |
| | ATOM | 1036 | O | PHE | A | 435 | 18.763 | 13.464 | 3.871 | 1.00 | 31.16 |
| | ATOM | 1037 | N | ARG | A | 436 | 16.812 | 14.137 | 2.975 | 1.00 | 33.37 |
| 30 | ATOM | 1038 | CA | ARG | A | 436 | 17.341 | 15.429 | 2.549 | 1.00 | 39.13 |
| | ATOM | 1039 | CB | ARG | A | 436 | 16.282 | 16.206 | 1.756 | 1.00 | 40.42 |
| | ATOM | 1040 | CG | ARG | A | 436 | 16.846 | 17.317 | 0.877 | 1.00 | 43.09 |
| | ATOM | 1041 | CD | ARG | A | 436 | 15.750 | 17.960 | 0.040 | 1.00 | 44.53 |
| | ATOM | 1042 | NE | ARG | A | 436 | 14.826 | 16.955 | -0.472 | 1.00 | 48.34 |
| 35 | ATOM | 1043 | CZ | ARG | A | 436 | 13.530 | 16.913 | -0.184 | 1.00 | 48.81 |
| | ATOM | 1044 | NH1 | ARG | A | 436 | 12.997 | 17.823 | 0.619 | 1.00 | 47.80 |
| | ATOM | 1045 | NH2 | ARG | A | 436 | 12.769 | 15.950 | -0.687 | 1.00 | 49.53 |
| | ATOM | 1046 | C | ARG | A | 436 | 17.792 | 16.250 | 3.753 | 1.00 | 38.10 |
| | ATOM | 1047 | O | ARG | A | 436 | 18.896 | 16.789 | 3.764 | 1.00 | 41.00 |
| 40 | ATOM | 1048 | N | MET | A | 437 | 16.936 | 16.334 | 4.766 | 1.00 | 39.47 |
| | ATOM | 1049 | CA | MET | A | 437 | 17.257 | 17.087 | 5.975 | 1.00 | 38.20 |
| | ATOM | 1050 | CB | MET | A | 437 | 16.102 | 16.998 | 6.965 | 1.00 | 39.79 |
| | ATOM | 1051 | C | MET | A | 437 | 18.550 | 16.594 | 6.626 | 1.00 | 41.15 |
| | ATOM | 1052 | O | MET | A | 437 | 19.303 | 17.378 | 7.201 | 1.00 | 40.20 |
| 45 | ATOM | 1053 | N | MET | A | 438 | 18.804 | 15.285 | 6.538 | 1.00 | 39.65 |
| | ATOM | 1054 | CA | MET | A | 438 | 20.011 | 14.693 | 7.117 | 1.00 | 39.70 |
| | ATOM | 1055 | CB | MET | A | 438 | 19.787 | 13.221 | 7.463 | 1.00 | 39.90 |
| | ATOM | 1056 | CG | MET | A | 438 | 18.694 | 12.938 | 8.460 | 1.00 | 41.94 |
| | ATOM | 1057 | SD | MET | A | 438 | 18.747 | 11.188 | 8.880 | 1.00 | 43.12 |
| 50 | ATOM | 1058 | CE | MET | A | 438 | 20.374 | 11.064 | 9.619 | 1.00 | 43.73 |
| | ATOM | 1059 | C | MET | A | 438 | 21.176 | 14.756 | 6.142 | 1.00 | 38.03 |
| | ATOM | 1060 | O | MET | A | 438 | 22.321 | 14.503 | 6.522 | 1.00 | 38.39 |
| | ATOM | 1061 | N | ASN | A | 439 | 20.886 | 15.070 | 4.895 | 1.00 | 37.64 |
| | ATOM | 1062 | CA | ASN | A | 439 | 21.924 | 15.118 | 3.895 | 1.00 | 35.68 |
| 55 | ATOM | 1063 | CB | ASN | A | 439 | 23.019 | 16.125 | 4.243 | 1.00 | 40.98 |
| | ATOM | 1064 | CG | ASN | A | 439 | 23.933 | 16.407 | 3.090 | 1.00 | 45.09 |
| | ATOM | 1065 | OD1 | ASN | A | 439 | 23.528 | 16.295 | 1.934 | 1.00 | 47.16 |
| | ATOM | 1066 | ND2 | ASN | A | 439 | 25.197 | 16.733 | 3.372 | 1.00 | 46.87 |
| | ATOM | 1067 | C | ASN | A | 439 | 22.552 | 13.732 | 3.739 | 1.00 | 31.06 |
| 60 | ATOM | 1068 | O | ASN | A | 439 | 23.764 | 13.581 | 3.649 | 1.00 | 29.54 |
| | ATOM | 1069 | N | LEU | A | 440 | 21.692 | 12.698 | 3.704 | 1.00 | 31.47 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1070 | CA | LEU | A | 440 | 22.161 | 11.326 | 3.579 | 1.00 | 31.63 |
| | ATOM | 1071 | CB | LEU | A | 440 | 20.991 | 10.344 | 3.380 | 1.00 | 33.05 |
| | ATOM | 1072 | CG | LEU | A | 440 | 21.451 | 8.886 | 3.209 | 1.00 | 37.07 |
| | ATOM | 1073 | CD1 | LEU | A | 440 | 21.957 | 8.353 | 4.546 | 1.00 | 36.18 |
| | ATOM | 1074 | CD2 | LEU | A | 440 | 20.318 | 8.032 | 2.682 | 1.00 | 32.33 |
| 10 | ATOM | 1075 | C | LEU | A | 440 | 23.146 | 11.161 | 2.435 | 1.00 | 32.10 |
| | ATOM | 1076 | O | LEU | A | 440 | 22.925 | 11.671 | 1.333 | 1.00 | 32.76 |
| | ATOM | 1077 | N | GLN | A | 441 | 24.225 | 10.450 | 2.702 | 1.00 | 32.54 |
| | ATOM | 1078 | CA | GLN | A | 441 | 25.255 | 10.220 | 1.699 | 1.00 | 31.97 |
| | ATOM | 1079 | CB | GLN | A | 441 | 26.632 | 10.320 | 2.345 | 1.00 | 31.75 |
| 15 | ATOM | 1080 | CG | GLN | A | 441 | 26.896 | 11.669 | 2.979 | 1.00 | 35.56 |
| | ATOM | 1081 | CD | GLN | A | 441 | 27.040 | 12.748 | 1.939 | 1.00 | 34.97 |
| | ATOM | 1082 | OE1 | GLN | A | 441 | 27.985 | 12.782 | 1.167 | 1.00 | 35.51 |
| | ATOM | 1083 | NE2 | GLN | A | 441 | 26.053 | 13.659 | 1.899 | 1.00 | 35.41 |
| | ATOM | 1084 | C | GLN | A | 441 | 25.100 | 8.860 | 1.038 | 1.00 | 34.08 |
| 20 | ATOM | 1085 | O | GLN | A | 441 | 24.540 | 7.931 | 1.625 | 1.00 | 30.73 |
| | ATOM | 1086 | N | GLY | A | 442 | 25.608 | 8.752 | -0.187 | 1.00 | 32.78 |
| | ATOM | 1087 | CA | GLY | A | 442 | 25.528 | 7.503 | -0.921 | 1.00 | 32.91 |
| | ATOM | 1088 | C | GLY | A | 442 | 26.181 | 6.350 | -0.184 | 1.00 | 31.87 |
| | ATOM | 1089 | O | GLY | A | 442 | 25.642 | 5.245 | -0.154 | 1.00 | 33.18 |
| 25 | ATOM | 1090 | N | GLU | A | 443 | 27.340 | 6.603 | 0.416 | 1.00 | 30.60 |
| | ATOM | 1091 | CA | GLU | A | 443 | 28.057 | 5.567 | 1.150 | 1.00 | 30.85 |
| | ATOM | 1092 | CB | GLU | A | 443 | 29.376 | 6.111 | 1.704 | 1.00 | 32.74 |
| | ATOM | 1093 | CG | GLU | A | 443 | 30.425 | 6.378 | 0.646 | 1.00 | 36.30 |
| | ATOM | 1094 | CD | GLU | A | 443 | 30.310 | 7.770 | 0.066 | 1.00 | 40.92 |
| 30 | ATOM | 1095 | OE1 | GLU | A | 443 | 29.677 | 8.630 | 0.716 | 1.00 | 42.27 |
| | ATOM | 1096 | OE2 | GLU | A | 443 | 30.853 | 8.003 | -1.038 | 1.00 | 46.82 |
| | ATOM | 1097 | C | GLU | A | 443 | 27.206 | 5.048 | 2.299 | 1.00 | 30.43 |
| | ATOM | 1098 | O | GLU | A | 443 | 27.211 | 3.854 | 2.595 | 1.00 | 28.11 |
| | ATOM | 1099 | N | GLU | A | 444 | 26.482 | 5.955 | 2.948 | 1.00 | 30.26 |
| 35 | ATOM | 1100 | CA | GLU | A | 444 | 25.619 | 5.589 | 4.067 | 1.00 | 28.18 |
| | ATOM | 1101 | CB | GLU | A | 444 | 25.147 | 6.843 | 4.797 | 1.00 | 26.32 |
| | ATOM | 1102 | CG | GLU | A | 444 | 26.250 | 7.633 | 5.463 | 1.00 | 29.27 |
| | ATOM | 1103 | CD | GLU | A | 444 | 25.748 | 8.944 | 6.023 | 1.00 | 29.62 |
| | ATOM | 1104 | OE1 | GLU | A | 444 | 25.006 | 9.652 | 5.304 | 1.00 | 32.00 |
| 40 | ATOM | 1105 | OE2 | GLU | A | 444 | 26.088 | 9.268 | 7.182 | 1.00 | 29.02 |
| | ATOM | 1106 | C | GLU | A | 444 | 24.403 | 4.813 | 3.572 | 1.00 | 26.93 |
| | ATOM | 1107 | O | GLU | A | 444 | 23.970 | 3.841 | 4.191 | 1.00 | 24.78 |
| | ATOM | 1108 | N | PHE | A | 445 | 23.861 | 5.256 | 2.443 | 1.00 | 27.79 |
| | ATOM | 1109 | CA | PHE | A | 445 | 22.688 | 4.633 | 1.853 | 1.00 | 24.50 |
| 45 | ATOM | 1110 | CB | PHE | A | 445 | 22.254 | 5.416 | 0.610 | 1.00 | 25.40 |
| | ATOM | 1111 | CG | PHE | A | 445 | 21.372 | 4.634 | -0.316 | 1.00 | 23.74 |
| | ATOM | 1112 | CD1 | PHE | A | 445 | 20.034 | 4.419 | -0.004 | 1.00 | 23.00 |
| | ATOM | 1113 | CD2 | PHE | A | 445 | 21.885 | 4.094 | -1.489 | 1.00 | 22.37 |
| | ATOM | 1114 | CE1 | PHE | A | 445 | 19.215 | 3.670 | -0.855 | 1.00 | 22.57 |
| 50 | ATOM | 1115 | CE2 | PHE | A | 445 | 21.079 | 3.349 | -2.342 | 1.00 | 21.69 |
| | ATOM | 1116 | CZ | PHE | A | 445 | 19.741 | 3.138 | -2.023 | 1.00 | 22.25 |
| | ATOM | 1117 | C | PHE | A | 445 | 22.913 | 3.169 | 1.489 | 1.00 | 22.81 |
| | ATOM | 1118 | O | PHE | A | 445 | 22.083 | 2.316 | 1.796 | 1.00 | 22.92 |
| | ATOM | 1119 | N | VAL | A | 446 | 24.019 | 2.868 | 0.822 | 1.00 | 22.46 |
| 55 | ATOM | 1120 | CA | VAL | A | 446 | 24.278 | 1.481 | 0.447 | 1.00 | 22.26 |
| | ATOM | 1121 | CB | VAL | A | 446 | 25.522 | 1.360 | -0.465 | 1.00 | 22.87 |
| | ATOM | 1122 | CG1 | VAL | A | 446 | 25.251 | 2.046 | -1.799 | 1.00 | 22.57 |
| | ATOM | 1123 | CG2 | VAL | A | 446 | 26.735 | 1.968 | 0.217 | 1.00 | 22.38 |
| | ATOM | 1124 | C | VAL | A | 446 | 24.467 | 0.614 | 1.694 | 1.00 | 23.68 |
| 60 | ATOM | 1125 | O | VAL | A | 446 | 24.177 | -0.586 | 1.680 | 1.00 | 22.91 |
| | ATOM | 1126 | N | CYS | A | 447 | 24.962 | 1.223 | 2.770 | 1.00 | 22.02 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1127 | CA | CYS | A | 447 | 25.155 | 0.503 | 4.025 | 1.00 | 24.17 |
| | ATOM | 1128 | CB | CYS | A | 447 | 25.953 | 1.359 | 5.011 | 1.00 | 23.95 |
| | ATOM | 1129 | SG | CYS | A | 447 | 27.738 | 1.324 | 4.731 | 1.00 | 28.57 |
| | ATOM | 1130 | C | CYS | A | 447 | 23.781 | 0.178 | 4.618 | 1.00 | 21.14 |
| | ATOM | 1131 | O | CYS | A | 447 | 23.512 | -0.960 | 5.002 | 1.00 | 19.37 |
| 10 | ATOM | 1132 | N | LEU | A | 448 | 22.915 | 1.186 | 4.680 | 1.00 | 19.28 |
| | ATOM | 1133 | CA | LEU | A | 448 | 21.568 | 1.002 | 5.219 | 1.00 | 21.31 |
| | ATOM | 1134 | CB | LEU | A | 448 | 20.803 | 2.324 | 5.207 | 1.00 | 21.90 |
| | ATOM | 1135 | CG | LEU | A | 448 | 21.142 | 3.337 | 6.303 | 1.00 | 26.61 |
| | ATOM | 1136 | CD1 | LEU | A | 448 | 20.328 | 4.594 | 6.072 | 1.00 | 27.74 |
| 15 | ATOM | 1137 | CD2 | LEU | A | 448 | 20.827 | 2.760 | 7.672 | 1.00 | 24.03 |
| | ATOM | 1138 | C | LEU | A | 448 | 20.766 | -0.038 | 4.442 | 1.00 | 21.72 |
| | ATOM | 1139 | O | LEU | A | 448 | 20.006 | -0.803 | 5.030 | 1.00 | 20.87 |
| | ATOM | 1140 | N | LYS | A | 449 | 20.929 | -0.055 | 3.119 | 1.00 | 21.42 |
| | ATOM | 1141 | CA | LYS | A | 449 | 20.205 | -0.997 | 2.269 | 1.00 | 20.98 |
| 20 | ATOM | 1142 | CB | LYS | A | 449 | 20.440 | -0.659 | 0.788 | 1.00 | 21.55 |
| | ATOM | 1143 | CG | LYS | A | 449 | 19.438 | -1.297 | -0.173 | 1.00 | 24.82 |
| | ATOM | 1144 | CD | LYS | A | 449 | 19.456 | -0.613 | -1.542 | 1.00 | 23.33 |
| | ATOM | 1145 | CE | LYS | A | 449 | 20.816 | -0.754 | -2.229 | 1.00 | 23.58 |
| | ATOM | 1146 | NZ | LYS | A | 449 | 20.741 | -0.482 | -3.698 | 1.00 | 28.77 |
| 25 | ATOM | 1147 | C | LYS | A | 449 | 20.629 | -2.436 | 2.548 | 1.00 | 20.33 |
| | ATOM | 1148 | O | LYS | A | 449 | 19.800 | -3.345 | 2.552 | 1.00 | 20.57 |
| | ATOM | 1149 | N | SER | A | 450 | 21.924 | -2.637 | 2.777 | 1.00 | 19.25 |
| | ATOM | 1150 | CA | SER | A | 450 | 22.451 | -3.965 | 3.074 | 1.00 | 21.84 |
| | ATOM | 1151 | CB | SER | A | 450 | 23.982 | -3.953 | 3.041 | 1.00 | 20.59 |
| 30 | ATOM | 1152 | OG | SER | A | 450 | 24.460 | -3.975 | 1.702 | 1.00 | 29.78 |
| | ATOM | 1153 | C | SER | A | 450 | 21.975 | -4.408 | 4.454 | 1.00 | 21.58 |
| | ATOM | 1154 | O | SER | A | 450 | 21.728 | -5.590 | 4.682 | 1.00 | 20.06 |
| | ATOM | 1155 | N | ILE | A | 451 | 21.853 | -3.449 | 5.369 | 1.00 | 22.20 |
| | ATOM | 1156 | CA | ILE | A | 451 | 21.385 | -3.741 | 6.726 | 1.00 | 22.82 |
| 35 | ATOM | 1157 | CB | ILE | A | 451 | 21.452 | -2.476 | 7.616 | 1.00 | 19.62 |
| | ATOM | 1158 | CG2 | ILE | A | 451 | 20.593 | -2.658 | 8.886 | 1.00 | 21.11 |
| | ATOM | 1159 | CG1 | ILE | A | 451 | 22.909 | -2.210 | 7.999 | 1.00 | 22.20 |
| | ATOM | 1160 | CD1 | ILE | A | 451 | 23.115 | -0.960 | 8.850 | 1.00 | 24.48 |
| | ATOM | 1161 | C | ILE | A | 451 | 19.952 | -4.250 | 6.662 | 1.00 | 21.82 |
| 40 | ATOM | 1162 | O | ILE | A | 451 | 19.575 | -5.184 | 7.369 | 1.00 | 21.72 |
| | ATOM | 1163 | N | ILE | A | 452 | 19.152 | -3.642 | 5.795 | 1.00 | 20.18 |
| | ATOM | 1164 | CA | ILE | A | 452 | 17.763 | -4.058 | 5.649 | 1.00 | 18.13 |
| | ATOM | 1165 | CB | ILE | A | 452 | 17.024 | -3.145 | 4.627 | 1.00 | 19.72 |
| | ATOM | 1166 | CG2 | ILE | A | 452 | 15.720 | -3.792 | 4.169 | 1.00 | 18.99 |
| 45 | ATOM | 1167 | CG1 | ILE | A | 452 | 16.725 | -1.788 | 5.282 | 1.00 | 18.33 |
| | ATOM | 1168 | CD1 | ILE | A | 452 | 16.284 | -0.707 | 4.306 | 1.00 | 23.25 |
| | ATOM | 1169 | C | ILE | A | 452 | 17.725 | -5.517 | 5.191 | 1.00 | 19.50 |
| | ATOM | 1170 | O | ILE | A | 452 | 16.980 | -6.340 | 5.737 | 1.00 | 17.60 |
| | ATOM | 1171 | N | LEU | A | 453 | 18.555 | -5.844 | 4.209 | 1.00 | 19.23 |
| 50 | ATOM | 1172 | CA | LEU | A | 453 | 18.589 | -7.205 | 3.679 | 1.00 | 21.60 |
| | ATOM | 1173 | CB | LEU | A | 453 | 19.624 | -7.316 | 2.554 | 1.00 | 21.50 |
| | ATOM | 1174 | CG | LEU | A | 453 | 19.835 | -8.729 | 1.989 | 1.00 | 25.06 |
| | ATOM | 1175 | CD1 | LEU | A | 453 | 18.550 | -9.250 | 1.364 | 1.00 | 25.27 |
| | ATOM | 1176 | CD2 | LEU | A | 453 | 20.948 | -8.694 | 0.953 | 1.00 | 24.73 |
| 55 | ATOM | 1177 | C | LEU | A | 453 | 18.906 | -8.245 | 4.746 | 1.00 | 19.41 |
| | ATOM | 1178 | O | LEU | A | 453 | 18.198 | -9.241 | 4.891 | 1.00 | 20.75 |
| | ATOM | 1179 | N | LEU | A | 454 | 19.966 | -7.997 | 5.499 | 1.00 | 21.35 |
| | ATOM | 1180 | CA | LEU | A | 454 | 20.410 | -8.925 | 6.530 | 1.00 | 23.67 |
| | ATOM | 1181 | CB | LEU | A | 454 | 21.870 | -8.625 | 6.878 | 1.00 | 20.69 |
| 60 | ATOM | 1182 | CG | LEU | A | 454 | 22.816 | -8.584 | 5.673 | 1.00 | 24.92 |
| | ATOM | 1183 | CD1 | LEU | A | 454 | 24.222 | -8.268 | 6.132 | 1.00 | 24.27 |

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 1184 | CD2 | LEU | A | 454 | 22.785 | -9.913 | 4.952 | 1.00 | 22.84 |
| | ATOM | 1185 | C | LEU | A | 454 | 19.572 | -8.945 | 7.807 | 1.00 | 26.06 |
| | ATOM | 1186 | O | LEU | A | 454 | 19.413 | -9.997 | 8.438 | 1.00 | 27.44 |
| | ATOM | 1187 | N | ASN | A | 455 | 19.011 | -7.795 | 8.167 | 1.00 | 25.01 |
| | ATOM | 1188 | CA | ASN | A | 455 | 18.240 | -7.681 | 9.400 | 1.00 | 26.10 |
| 10 | ATOM | 1189 | CB | ASN | A | 455 | 18.439 | -6.295 | 10.002 | 1.00 | 22.67 |
| | ATOM | 1190 | CG | ASN | A | 455 | 17.627 | -6.109 | 11.264 | 1.00 | 26.67 |
| | ATOM | 1191 | OD1 | ASN | A | 455 | 17.899 | -6.751 | 12.270 | 1.00 | 25.16 |
| | ATOM | 1192 | ND2 | ASN | A | 455 | 16.615 | -5.246 | 11.212 | 1.00 | 20.73 |
| | ATOM | 1193 | C | ASN | A | 455 | 16.739 | -7.957 | 9.418 | 1.00 | 25.78 |
| 15 | ATOM | 1194 | O | ASN | A | 455 | 16.230 | -8.516 | 10.380 | 1.00 | 29.22 |
| | ATOM | 1195 | N | SER | A | 456 | 16.027 | -7.549 | 8.381 | 1.00 | 28.51 |
| | ATOM | 1196 | CA | SER | A | 456 | 14.578 | -7.704 | 8.371 | 1.00 | 32.52 |
| | ATOM | 1197 | CB | SER | A | 456 | 14.019 | -7.213 | 7.033 | 1.00 | 35.98 |
| | ATOM | 1198 | OG | SER | A | 456 | 14.266 | -5.818 | 6.897 | 1.00 | 30.88 |
| 20 | ATOM | 1199 | C | SER | A | 456 | 14.033 | -9.086 | 8.711 | 1.00 | 33.00 |
| | ATOM | 1200 | O | SER | A | 456 | 13.112 | -9.202 | 9.523 | 1.00 | 33.07 |
| | ATOM | 1201 | N | GLY | A | 457 | 14.597 | -10.130 | 8.117 | 1.00 | 28.40 |
| | ATOM | 1202 | CA | GLY | A | 457 | 14.115 | -11.464 | 8.413 | 1.00 | 36.28 |
| | ATOM | 1203 | C | GLY | A | 457 | 15.055 | -12.289 | 9.277 | 1.00 | 40.41 |
| 25 | ATOM | 1204 | O | GLY | A | 457 | 14.831 | -13.486 | 9.456 | 1.00 | 38.20 |
| | ATOM | 1205 | N | VAL | A | 458 | 16.095 | -11.657 | 9.820 | 1.00 | 44.13 |
| | ATOM | 1206 | CA | VAL | A | 458 | 17.079 | -12.356 | 10.647 | 1.00 | 51.09 |
| | ATOM | 1207 | CB | VAL | A | 458 | 18.214 | -11.399 | 11.095 | 1.00 | 51.06 |
| | ATOM | 1208 | CG1 | VAL | A | 458 | 17.688 | -10.390 | 12.104 | 1.00 | 51.75 |
| 30 | ATOM | 1209 | CG2 | VAL | A | 458 | 19.365 | -12.199 | 11.692 | 1.00 | 50.65 |
| | ATOM | 1210 | C | VAL | A | 458 | 16.513 | -13.060 | 11.885 | 1.00 | 57.26 |
| | ATOM | 1211 | O | VAL | A | 458 | 17.085 | -14.045 | 12.356 | 1.00 | 58.77 |
| | ATOM | 1212 | N | TYR | A | 459 | 15.401 | -12.560 | 12.416 | 1.00 | 62.31 |
| | ATOM | 1213 | CA | TYR | A | 459 | 14.793 | -13.177 | 13.592 | 1.00 | 68.49 |
| 35 | ATOM | 1214 | CB | TYR | A | 459 | 14.293 | -12.100 | 14.560 | 1.00 | 70.46 |
| | ATOM | 1215 | CG | TYR | A | 459 | 15.396 | -11.196 | 15.069 | 1.00 | 71.73 |
| | ATOM | 1216 | CD1 | TYR | A | 459 | 15.127 | -9.888 | 15.462 | 1.00 | 71.93 |
| | ATOM | 1217 | CE1 | TYR | A | 459 | 16.147 | -9.045 | 15.898 | 1.00 | 72.60 |
| | ATOM | 1218 | CD2 | TYR | A | 459 | 16.716 | -11.644 | 15.128 | 1.00 | 72.77 |
| 40 | ATOM | 1219 | CE2 | TYR | A | 459 | 17.741 | -10.812 | 15.560 | 1.00 | 73.55 |
| | ATOM | 1220 | CZ | TYR | A | 459 | 17.450 | -9.514 | 15.941 | 1.00 | 72.93 |
| | ATOM | 1221 | OH | TYR | A | 459 | 18.467 | -8.687 | 16.351 | 1.00 | 74.56 |
| | ATOM | 1222 | C | TYR | A | 459 | 13.649 | -14.097 | 13.187 | 1.00 | 71.86 |
| | ATOM | 1223 | O | TYR | A | 459 | 13.380 | -15.099 | 13.852 | 1.00 | 73.11 |
| 45 | ATOM | 1224 | N | THR | A | 460 | 12.981 | -13.756 | 12.090 | 1.00 | 74.84 |
| | ATOM | 1225 | CA | THR | A | 460 | 11.881 | -14.567 | 11.589 | 1.00 | 77.66 |
| | ATOM | 1226 | CB | THR | A | 460 | 11.246 | -13.900 | 10.373 | 1.00 | 76.69 |
| | ATOM | 1227 | C | THR | A | 460 | 12.436 | -15.938 | 11.212 | 1.00 | 80.26 |
| | ATOM | 1228 | O | THR | A | 460 | 11.684 | -16.866 | 10.912 | 1.00 | 80.82 |
| 50 | ATOM | 1229 | N | PHE | A | 461 | 13.762 | -16.051 | 11.231 | 1.00 | 82.69 |
| | ATOM | 1230 | CA | PHE | A | 461 | 14.440 | -17.299 | 10.905 | 1.00 | 85.63 |
| | ATOM | 1231 | CB | PHE | A | 461 | 15.920 | -17.034 | 10.630 | 1.00 | 85.47 |
| | ATOM | 1232 | C | PHE | A | 461 | 14.284 | -18.288 | 12.059 | 1.00 | 87.52 |
| | ATOM | 1233 | O | PHE | A | 461 | 14.493 | -17.940 | 13.224 | 1.00 | 86.53 |
| 55 | ATOM | 1234 | N | LEU | A | 462 | 13.914 | -19.520 | 11.724 | 1.00 | 89.49 |
| | ATOM | 1235 | CA | LEU | A | 462 | 13.711 | -20.568 | 12.718 | 1.00 | 91.34 |
| | ATOM | 1236 | CB | LEU | A | 462 | 12.961 | -21.741 | 12.087 | 1.00 | 91.23 |
| | ATOM | 1237 | C | LEU | A | 462 | 15.016 | -21.060 | 13.340 | 1.00 | 92.05 |
| | ATOM | 1238 | O | LEU | A | 462 | 16.042 | -21.165 | 12.664 | 1.00 | 91.91 |
| 60 | ATOM | 1239 | N | SER | A | 463 | 14.966 | -21.357 | 14.635 | 1.00 | 92.53 |
| | ATOM | 1240 | CA | SER | A | 463 | 16.131 | -21.855 | 15.358 | 1.00 | 92.96 |

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 1241 | CB | SER | A | 463 | 16.033 | -21.483 | 16.833 | 1.00 | 91.67 |
| | ATOM | 1242 | C | SER | A | 463 | 16.189 | -23.371 | 15.200 | 1.00 | 93.39 |
| | ATOM | 1243 | O | SER | A | 463 | 15.156 | -24.034 | 15.102 | 1.00 | 93.44 |
| | ATOM | 1244 | N | SER | A | 464 | 17.399 | -23.917 | 15.167 | 1.00 | 93.82 |
| | ATOM | 1245 | CA | SER | A | 464 | 17.577 | -25.355 | 15.015 | 1.00 | 93.85 |
| 10 | ATOM | 1246 | CB | SER | A | 464 | 17.284 | -25.769 | 13.577 | 1.00 | 93.74 |
| | ATOM | 1247 | C | SER | A | 464 | 18.997 | -25.743 | 15.396 | 1.00 | 93.96 |
| | ATOM | 1248 | O | SER | A | 464 | 19.815 | -26.074 | 14.535 | 1.00 | 93.65 |
| | ATOM | 1249 | N | THR | A | 465 | 19.279 | -25.699 | 16.694 | 1.00 | 93.91 |
| | ATOM | 1250 | CA | THR | A | 465 | 20.600 | -26.036 | 17.212 | 1.00 | 93.79 |
| 15 | ATOM | 1251 | CB | THR | A | 465 | 20.952 | -27.483 | 16.863 | 1.00 | 93.38 |
| | ATOM | 1252 | C | THR | A | 465 | 21.640 | -25.085 | 16.634 | 1.00 | 93.27 |
| | ATOM | 1253 | O | THR | A | 465 | 21.302 | -24.017 | 16.121 | 1.00 | 93.03 |
| | ATOM | 1254 | N | LEU | A | 466 | 22.907 | -25.479 | 16.723 | 1.00 | 93.26 |
| | ATOM | 1255 | CA | LEU | A | 466 | 23.999 | -24.665 | 16.207 | 1.00 | 92.34 |
| 20 | ATOM | 1256 | CB | LEU | A | 466 | 25.335 | -25.338 | 16.498 | 1.00 | 91.59 |
| | ATOM | 1257 | C | LEU | A | 466 | 23.829 | -24.461 | 14.706 | 1.00 | 92.18 |
| | ATOM | 1258 | O | LEU | A | 466 | 24.411 | -23.545 | 14.125 | 1.00 | 92.67 |
| | ATOM | 1259 | N | LYS | A | 467 | 23.028 | -25.323 | 14.086 | 1.00 | 91.28 |
| | ATOM | 1260 | CA | LYS | A | 467 | 22.772 | -25.238 | 12.653 | 1.00 | 90.02 |
| 25 | ATOM | 1261 | CB | LYS | A | 467 | 21.740 | -26.287 | 12.240 | 1.00 | 89.93 |
| | ATOM | 1262 | C | LYS | A | 467 | 22.269 | -23.841 | 12.308 | 1.00 | 88.35 |
| | ATOM | 1263 | O | LYS | A | 467 | 23.032 | -22.990 | 11.849 | 1.00 | 88.50 |
| | ATOM | 1264 | N | SER | A | 468 | 20.981 | -23.610 | 12.536 | 1.00 | 86.02 |
| | ATOM | 1265 | CA | SER | A | 468 | 20.384 | -22.315 | 12.252 | 1.00 | 84.10 |
| 30 | ATOM | 1266 | CB | SER | A | 468 | 18.901 | -22.333 | 12.620 | 1.00 | 84.08 |
| | ATOM | 1267 | OG | SER | A | 468 | 18.229 | -23.378 | 11.937 | 1.00 | 83.03 |
| | ATOM | 1268 | C | SER | A | 468 | 21.109 | -21.230 | 13.040 | 1.00 | 83.39 |
| | ATOM | 1269 | O | SER | A | 468 | 21.264 | -20.105 | 12.565 | 1.00 | 83.48 |
| | ATOM | 1270 | N | LEU | A | 469 | 21.558 | -21.579 | 14.242 | 1.00 | 82.04 |
| 35 | ATOM | 1271 | CA | LEU | A | 469 | 22.276 | -20.640 | 15.098 | 1.00 | 80.28 |
| | ATOM | 1272 | CB | LEU | A | 469 | 22.595 | -21.294 | 16.436 | 1.00 | 79.81 |
| | ATOM | 1273 | C | LEU | A | 469 | 23.564 | -20.174 | 14.419 | 1.00 | 79.18 |
| | ATOM | 1274 | O | LEU | A | 469 | 24.111 | -19.122 | 14.756 | 1.00 | 78.61 |
| | ATOM | 1275 | N | GLU | A | 470 | 24.044 | -20.969 | 13.466 | 1.00 | 76.69 |
| 40 | ATOM | 1276 | CA | GLU | A | 470 | 25.256 | -20.638 | 12.726 | 1.00 | 74.84 |
| | ATOM | 1277 | CB | GLU | A | 470 | 25.803 | -21.880 | 12.032 | 1.00 | 74.12 |
| | ATOM | 1278 | C | GLU | A | 470 | 24.920 | -19.565 | 11.697 | 1.00 | 73.77 |
| | ATOM | 1279 | O | GLU | A | 470 | 25.617 | -18.556 | 11.581 | 1.00 | 72.94 |
| | ATOM | 1280 | N | GLU | A | 471 | 23.842 | -19.792 | 10.953 | 1.00 | 72.08 |
| 45 | ATOM | 1281 | CA | GLU | A | 471 | 23.396 | -18.842 | 9.945 | 1.00 | 70.05 |
| | ATOM | 1282 | CB | GLU | A | 471 | 22.461 | -19.526 | 8.944 | 1.00 | 71.52 |
| | ATOM | 1283 | CG | GLU | A | 471 | 23.150 | -19.976 | 7.668 | 1.00 | 72.90 |
| | ATOM | 1284 | CD | GLU | A | 471 | 24.512 | -20.586 | 7.932 | 1.00 | 74.01 |
| | ATOM | 1285 | OE1 | GLU | A | 471 | 25.469 | -20.258 | 7.198 | 1.00 | 74.22 |
| 50 | ATOM | 1286 | OE2 | GLU | A | 471 | 24.626 | -21.395 | 8.878 | 1.00 | 75.18 |
| | ATOM | 1287 | C | GLU | A | 471 | 22.667 | -17.692 | 10.630 | 1.00 | 67.33 |
| | ATOM | 1288 | O | GLU | A | 471 | 21.685 | -17.165 | 10.107 | 1.00 | 67.77 |
| | ATOM | 1289 | N | LYS | A | 472 | 23.152 | -17.319 | 11.811 | 1.00 | 62.63 |
| | ATOM | 1290 | CA | LYS | A | 472 | 22.564 | -16.229 | 12.578 | 1.00 | 57.41 |
| 55 | ATOM | 1291 | CB | LYS | A | 472 | 21.697 | -16.777 | 13.713 | 1.00 | 58.74 |
| | ATOM | 1292 | CG | LYS | A | 472 | 20.683 | -15.776 | 14.243 | 1.00 | 60.32 |
| | ATOM | 1293 | CD | LYS | A | 472 | 19.271 | -16.342 | 14.219 | 1.00 | 60.73 |
| | ATOM | 1294 | CE | LYS | A | 472 | 18.485 | -15.909 | 15.449 | 1.00 | 61.78 |
| | ATOM | 1295 | NZ | LYS | A | 472 | 19.352 | -15.788 | 16.658 | 1.00 | 60.09 |
| 60 | ATOM | 1296 | C | LYS | A | 472 | 23.662 | -15.339 | 13.150 | 1.00 | 53.42 |
| | ATOM | 1297 | O | LYS | A | 472 | 23.631 | -14.120 | 12.978 | 1.00 | 50.87 |

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 1298 | N | ASP | A | 473 | 24.628 | -15.949 | 13.830 | 1.00 | 47.52 |
| | ATOM | 1299 | CA | ASP | A | 473 | 25.732 | -15.194 | 14.405 | 1.00 | 45.55 |
| | ATOM | 1300 | CB | ASP | A | 473 | 26.613 | -16.094 | 15.269 | 1.00 | 50.48 |
| | ATOM | 1301 | CG | ASP | A | 473 | 26.380 | -15.885 | 16.749 | 1.00 | 55.50 |
| | ATOM | 1302 | OD1 | ASP | A | 473 | 25.272 | -15.436 | 17.118 | 1.00 | 58.06 |
| 10 | ATOM | 1303 | OD2 | ASP | A | 473 | 27.304 | -16.170 | 17.541 | 1.00 | 59.81 |
| | ATOM | 1304 | C | ASP | A | 473 | 26.557 | -14.611 | 13.269 | 1.00 | 42.62 |
| | ATOM | 1305 | O | ASP | A | 473 | 27.087 | -13.506 | 13.373 | 1.00 | 42.10 |
| | ATOM | 1306 | N | HIS | A | 474 | 26.663 | -15.364 | 12.180 | 1.00 | 38.05 |
| | ATOM | 1307 | CA | HIS | A | 474 | 27.416 | -14.904 | 11.026 | 1.00 | 37.25 |
| 15 | ATOM | 1308 | CB | HIS | A | 474 | 27.429 | -15.978 | 9.941 | 1.00 | 35.07 |
| | ATOM | 1309 | CG | HIS | A | 474 | 28.036 | -15.523 | 8.653 | 1.00 | 37.36 |
| | ATOM | 1310 | CD2 | HIS | A | 474 | 29.292 | -15.113 | 8.355 | 1.00 | 38.86 |
| | ATOM | 1311 | ND1 | HIS | A | 474 | 27.322 | -15.452 | 7.476 | 1.00 | 41.31 |
| | ATOM | 1312 | CE1 | HIS | A | 474 | 28.110 | -15.020 | 6.509 | 1.00 | 40.86 |
| 20 | ATOM | 1313 | NE2 | HIS | A | 474 | 29.311 | -14.807 | 7.016 | 1.00 | 44.49 |
| | ATOM | 1314 | C | HIS | A | 474 | 26.749 | -13.640 | 10.493 | 1.00 | 36.68 |
| | ATOM | 1315 | O | HIS | A | 474 | 27.417 | -12.676 | 10.132 | 1.00 | 36.48 |
| | ATOM | 1316 | N | ILE | A | 475 | 25.422 | -13.652 | 10.447 | 1.00 | 35.93 |
| | ATOM | 1317 | CA | ILE | A | 475 | 24.683 | -12.499 | 9.963 | 1.00 | 36.21 |
| 25 | ATOM | 1318 | CB | ILE | A | 475 | 23.174 | -12.797 | 9.868 | 1.00 | 36.31 |
| | ATOM | 1319 | CG2 | ILE | A | 475 | 22.411 | -11.527 | 9.513 | 1.00 | 38.19 |
| | ATOM | 1320 | CG1 | ILE | A | 475 | 22.922 | -13.874 | 8.813 | 1.00 | 36.97 |
| | ATOM | 1321 | CD1 | ILE | A | 475 | 21.528 | -14.454 | 8.869 | 1.00 | 35.59 |
| | ATOM | 1322 | C | ILE | A | 475 | 24.893 | -11.322 | 10.907 | 1.00 | 35.34 |
| 30 | ATOM | 1323 | O | ILE | A | 475 | 25.092 | -10.189 | 10.471 | 1.00 | 33.20 |
| | ATOM | 1324 | N | HIS | A | 476 | 24.857 | -11.596 | 12.206 | 1.00 | 35.95 |
| | ATOM | 1325 | CA | HIS | A | 476 | 25.031 | -10.540 | 13.193 | 1.00 | 35.06 |
| | ATOM | 1326 | CB | HIS | A | 476 | 24.681 | -11.062 | 14.585 | 1.00 | 37.30 |
| | ATOM | 1327 | CG | HIS | A | 476 | 23.210 | -11.068 | 14.860 | 1.00 | 43.06 |
| 35 | ATOM | 1328 | CD2 | HIS | A | 476 | 22.329 | -10.051 | 15.017 | 1.00 | 43.93 |
| | ATOM | 1329 | ND1 | HIS | A | 476 | 22.476 | -12.230 | 14.968 | 1.00 | 45.60 |
| | ATOM | 1330 | CE1 | HIS | A | 476 | 21.207 | -11.928 | 15.177 | 1.00 | 47.56 |
| | ATOM | 1331 | NE2 | HIS | A | 476 | 21.091 | -10.613 | 15.211 | 1.00 | 46.21 |
| | ATOM | 1332 | C | HIS | A | 476 | 26.438 | -9.966 | 13.170 | 1.00 | 35.40 |
| 40 | ATOM | 1333 | O | HIS | A | 476 | 26.634 | -8.774 | 13.415 | 1.00 | 35.45 |
| | ATOM | 1334 | N | ARG | A | 477 | 27.420 | -10.805 | 12.862 | 1.00 | 34.07 |
| | ATOM | 1335 | CA | ARG | A | 477 | 28.796 | -10.331 | 12.795 | 1.00 | 34.18 |
| | ATOM | 1336 | CB | ARG | A | 477 | 29.757 | -11.506 | 12.605 | 1.00 | 41.04 |
| | ATOM | 1337 | CG | ARG | A | 477 | 29.800 | -12.459 | 13.788 | 1.00 | 47.61 |
| 45 | ATOM | 1338 | CD | ARG | A | 477 | 30.782 | -13.599 | 13.557 | 1.00 | 55.67 |
| | ATOM | 1339 | NE | ARG | A | 477 | 31.780 | -13.675 | 14.622 | 1.00 | 60.17 |
| | ATOM | 1340 | CZ | ARG | A | 477 | 32.780 | -12.811 | 14.770 | 1.00 | 61.98 |
| | ATOM | 1341 | NH1 | ARG | A | 477 | 32.918 | -11.803 | 13.918 | 1.00 | 64.29 |
| | ATOM | 1342 | NH2 | ARG | A | 477 | 33.643 | -12.955 | 15.766 | 1.00 | 62.79 |
| 50 | ATOM | 1343 | C | ARG | A | 477 | 28.906 | -9.361 | 11.621 | 1.00 | 30.77 |
| | ATOM | 1344 | O | ARG | A | 477 | 29.462 | -8.268 | 11.753 | 1.00 | 33.59 |
| | ATOM | 1345 | N | VAL | A | 478 | 28.369 | -9.766 | 10.475 | 1.00 | 27.65 |
| | ATOM | 1346 | CA | VAL | A | 478 | 28.389 | -8.930 | 9.280 | 1.00 | 27.07 |
| | ATOM | 1347 | CB | VAL | A | 478 | 27.658 | -9.605 | 8.100 | 1.00 | 28.00 |
| 55 | ATOM | 1348 | CG1 | VAL | A | 478 | 27.672 | -8.678 | 6.890 | 1.00 | 25.83 |
| | ATOM | 1349 | CG2 | VAL | A | 478 | 28.319 | -10.933 | 7.761 | 1.00 | 31.66 |
| | ATOM | 1350 | C | VAL | A | 478 | 27.689 | -7.610 | 9.584 | 1.00 | 26.92 |
| | ATOM | 1351 | O | VAL | A | 478 | 28.216 | -6.536 | 9.294 | 1.00 | 26.97 |
| | ATOM | 1352 | N | LEU | A | 479 | 26.499 | -7.702 | 10.171 | 1.00 | 25.74 |
| 60 | ATOM | 1353 | CA | LEU | A | 479 | 25.727 | -6.516 | 10.530 | 1.00 | 27.97 |
| | ATOM | 1354 | CB | LEU | A | 479 | 24.474 | -6.912 | 11.324 | 1.00 | 25.55 |

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|----|------|------|-----|-----|---|-----|--------|-------------------|--------|------|-------|
| 5 | ATOM | 1355 | CG | LEU | A | 479 | 23.211 | 27.229 | 10.517 | 1.00 | 29.01 |
| | ATOM | 1356 | CD1 | LEU | A | 479 | 22.056 | -7.503 | 11.481 | 1.00 | 27.05 |
| | ATOM | 1357 | CD2 | LEU | A | 479 | 22.864 | -6.063 | 9.584 | 1.00 | 24.92 |
| | ATOM | 1358 | C | LEU | A | 479 | 26.592 | -5.582 | 11.369 | 1.00 | 25.39 |
| | ATOM | 1359 | O | LEU | A | 479 | 26.595 | -4.370 | 11.158 | 1.00 | 27.39 |
| 10 | ATOM | 1360 | N | ASP | A | 480 | 27.324 | -6.158 | 12.320 | 1.00 | 26.04 |
| | ATOM | 1361 | CA | ASP | A | 480 | 28.206 | -5.388 | 13.193 | 1.00 | 27.32 |
| | ATOM | 1362 | CB | ASP | A | 480 | 28.878 | -6.305 | 14.222 | 1.00 | 26.67 |
| | ATOM | 1363 | CG | ASP | A | 480 | 27.990 | -6.602 | 15.417 | 1.00 | 31.02 |
| | ATOM | 1364 | OD1 | ASP | A | 480 | 28.355 | -7.505 | 16.198 | 1.00 | 31.50 |
| 15 | ATOM | 1365 | OD2 | ASP | A | 480 | 26.935 | -5.944 | 15.580 | 1.00 | 32.21 |
| | ATOM | 1366 | C | ASP | A | 480 | 29.283 | -4.699 | 12.361 | 1.00 | 25.59 |
| | ATOM | 1367 | O | ASP | A | 480 | 29.672 | -3.562 | 12.636 | 1.00 | 27.15 |
| | ATOM | 1368 | N | LYS | A | 481 | 29.767 | -5.394 | 11.340 | 1.00 | 25.17 |
| | ATOM | 1369 | CA | LYS | A | 481 | 30.794 | -4.830 | 10.477 | 1.00 | 24.93 |
| 20 | ATOM | 1370 | CB | LYS | A | 481 | 31.306 | -5.890 | 9.512 | 1.00 | 28.42 |
| | ATOM | 1371 | CG | LYS | A | 481 | 32.158 | -6.953 | 10.188 | 1.00 | 35.59 |
| | ATOM | 1372 | CD | LYS | A | 481 | 32.894 | -7.799 | 9.157 | 1.00 | 41.21 |
| | ATOM | 1373 | CE | LYS | A | 481 | 33.883 | -6.963 | 8.350 | 1.00 | 41.48 |
| | ATOM | 1374 | NZ | LYS | A | 481 | 34.954 | -6.388 | 9.215 | 1.00 | 43.22 |
| 25 | ATOM | 1375 | C | LYS | A | 481 | 30.260 | -3.635 | 9.696 | 1.00 | 26.12 |
| | ATOM | 1376 | O | LYS | A | 481 | 30.979 | -2.657 | 9.463 | 1.00 | 23.73 |
| | ATOM | 1377 | N | ILE | A | 482 | 28.996 | -3.705 | 9.291 | 1.00 | 25.44 |
| | ATOM | 1378 | CA | ILE | A | 482 | 28.421 | -2.598 | 8.545 | 1.00 | 27.69 |
| | ATOM | 1379 | CB | ILE | A | 482 | 27.066 | -2.983 | 7.915 | 1.00 | 27.59 |
| 30 | ATOM | 1380 | CG2 | ILE | A | 482 | 26.470 | -1.788 | 7.183 | 1.00 | 25.97 |
| | ATOM | 1381 | CG1 | ILE | A | 482 | 27.274 | -4.131 | 6.922 | 1.00 | 23.80 |
| | ATOM | 1382 | CD1 | ILE | A | 482 | 26.000 | -4.838 | 6.533 | 1.00 | 21.30 |
| | ATOM | 1383 | C | ILE | A | 482 | 28.253 | -1.408 | 9.481 | 1.00 | 27.33 |
| | ATOM | 1384 | O | ILE | A | 482 | 28.312 | -0.256 | 9.045 | 1.00 | 28.55 |
| 35 | ATOM | 1385 | N | THR | A | 483 | 28.046 | -1.690 | 10.768 | 1.00 | 25.03 |
| | ATOM | 1386 | CA | THR | A | 483 | 27.905 | -0.632 | 11.760 | 1.00 | 23.62 |
| | ATOM | 1387 | CB | THR | A | 483 | 27.535 | -1.192 | 13.154 | 1.00 | 22.18 |
| | ATOM | 1388 | OG1 | THR | A | 483 | 26.181 | -1.658 | 13.133 | 1.00 | 25.39 |
| | ATOM | 1389 | CG2 | THR | A | 483 | 27.673 | -0.111 | 14.226 | 1.00 | 25.84 |
| 40 | ATOM | 1390 | C | THR | A | 483 | 29.257 | 0.074 | 11.858 | 1.00 | 23.04 |
| | ATOM | 1391 | O | THR | A | 483 | 29.331 | 1.306 | 11.846 | 1.00 | 23.55 |
| | ATOM | 1392 | N | ASP | A | 484 | 30.324 | -0.714 | 11.960 | 1.00 | 22.24 |
| | ATOM | 1393 | CA | ASP | A | 484 | 31.674 | -0.152 | 12.039 | 1.00 | 25.48 |
| | ATOM | 1394 | CB | ASP | A | 484 | 32.718 | -1.273 | 12.107 | 1.00 | 26.88 |
| 45 | ATOM | 1395 | CG | ASP | A | 484 | 32.629 | -2.083 | 13.394 | 1.00 | 32.52 |
| | ATOM | 1396 | OD1 | ASP | A | 484 | 32.002 | -1.608 | 14.366 | 1.00 | 33.68 |
| | ATOM | 1397 | OD2 | ASP | A | 484 | 33.185 | -3.198 | 13.434 | 1.00 | 34.63 |
| | ATOM | 1398 | C | ASP | A | 484 | 31.930 | 0.715 | 10.807 | 1.00 | 25.16 |
| | ATOM | 1399 | O | ASP | A | 484 | 32.481 | 1.812 | 10.905 | 1.00 | 26.05 |
| 50 | ATOM | 1400 | N | THR | A | 485 | 31.505 | 0.226 | 9.645 | 1.00 | 28.96 |
| | ATOM | 1401 | CA | THR | A | 485 | 31.689 | 0.960 | 8.394 | 1.00 | 26.63 |
| | ATOM | 1402 | CB | THR | A | 485 | 31.124 | 0.166 | 7.197 | 1.00 | 26.12 |
| | ATOM | 1403 | OG1 | THR | A | 485 | 31.753 | -1.123 | 7.132 | 1.00 | 24.30 |
| | ATOM | 1404 | CG2 | THR | A | 485 | 31.381 | 0.907 | 5.898 | 1.00 | 23.31 |
| 55 | ATOM | 1405 | C | THR | A | 485 | 30.994 | 2.318 | 8.468 | 1.00 | 28.90 |
| | ATOM | 1406 | O | THR | A | 485 | 31.583 | 3.354 | 8.137 | 1.00 | 27.26 |
| | ATOM | 1407 | N | LEU | A | 486 | 29.743 | 2.310 | 8.915 | 1.00 | 24.76 |
| | ATOM | 1408 | CA | LEU | A | 486 | 28.973 | 3.537 | 9.027 | 1.00 | 26.19 |
| | ATOM | 1409 | CB | LEU | A | 486 | 27.567 | 3.233 | 9.547 | 1.00 | 27.27 |
| 60 | ATOM | 1410 | CG | LEU | A | 486 | 26.508 | 2.921 | 8.486 | 1.00 | 23.50 |
| | ATOM | 1411 | CD1 | LEU | A | 486 | 25.210 | 2.550 | 9.183 | 1.00 | 22.03 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1412 | CD2 | LEU | A | 486 | 26.309 | 4.128 | 7.577 | 1.00 | 21.35 |
| | ATOM | 1413 | C | LEU | A | 486 | 29.662 | 4.519 | 9.960 | 1.00 | 27.36 |
| | ATOM | 1414 | O | LEU | A | 486 | 29.745 | 5.710 | 9.669 | 1.00 | 25.87 |
| | ATOM | 1415 | N | ILE | A | 487 | 30.151 | 4.015 | 11.088 | 1.00 | 27.88 |
| | ATOM | 1416 | CA | ILE | A | 487 | 30.843 | 4.857 | 12.055 | 1.00 | 28.40 |
| 10 | ATOM | 1417 | CB | ILE | A | 487 | 31.203 | 4.054 | 13.332 | 1.00 | 26.74 |
| | ATOM | 1418 | CG2 | ILE | A | 487 | 32.255 | 4.803 | 14.154 | 1.00 | 27.54 |
| | ATOM | 1419 | CG1 | ILE | A | 487 | 29.937 | 3.813 | 14.163 | 1.00 | 25.93 |
| | ATOM | 1420 | CD1 | ILE | A | 487 | 29.237 | 5.088 | 14.624 | 1.00 | 23.42 |
| | ATOM | 1421 | C | ILE | A | 487 | 32.125 | 5.393 | 11.412 | 1.00 | 28.89 |
| 15 | ATOM | 1422 | O | ILE | A | 487 | 32.497 | 6.554 | 11.602 | 1.00 | 29.85 |
| | ATOM | 1423 | N | HIS | A | 488 | 32.791 | 4.533 | 10.649 | 1.00 | 29.71 |
| | ATOM | 1424 | CA | HIS | A | 488 | 34.031 | 4.898 | 9.967 | 1.00 | 34.12 |
| | ATOM | 1425 | CB | HIS | A | 488 | 34.585 | 3.691 | 9.207 | 1.00 | 36.61 |
| | ATOM | 1426 | CG | HIS | A | 488 | 35.799 | 3.997 | 8.385 | 1.00 | 42.74 |
| 20 | ATOM | 1427 | CD2 | HIS | A | 488 | 35.970 | 4.089 | 7.045 | 1.00 | 43.12 |
| | ATOM | 1428 | ND1 | HIS | A | 488 | 37.034 | 4.239 | 8.946 | 1.00 | 43.13 |
| | ATOM | 1429 | CE1 | HIS | A | 488 | 37.913 | 4.466 | 7.987 | 1.00 | 43.40 |
| | ATOM | 1430 | NE2 | HIS | A | 488 | 37.293 | 4.381 | 6.825 | 1.00 | 45.63 |
| | ATOM | 1431 | C | HIS | A | 488 | 33.799 | 6.051 | 8.998 | 1.00 | 32.74 |
| 25 | ATOM | 1432 | O | HIS | A | 488 | 34.577 | 7.004 | 8.955 | 1.00 | 31.06 |
| | ATOM | 1433 | N | LEU | A | 489 | 32.721 | 5.958 | 8.223 | 1.00 | 33.56 |
| | ATOM | 1434 | CA | LEU | A | 489 | 32.384 | 6.992 | 7.258 | 1.00 | 30.78 |
| | ATOM | 1435 | CB | LEU | A | 489 | 31.145 | 6.587 | 6.464 | 1.00 | 34.67 |
| | ATOM | 1436 | CG | LEU | A | 489 | 31.310 | 5.353 | 5.574 | 1.00 | 34.73 |
| 30 | ATOM | 1437 | CD1 | LEU | A | 489 | 29.945 | 4.856 | 5.125 | 1.00 | 33.21 |
| | ATOM | 1438 | CD2 | LEU | A | 489 | 32.183 | 5.701 | 4.378 | 1.00 | 35.92 |
| | ATOM | 1439 | C | LEU | A | 489 | 32.124 | 8.320 | 7.954 | 1.00 | 33.97 |
| | ATOM | 1440 | O | LEU | A | 489 | 32.587 | 9.365 | 7.507 | 1.00 | 33.22 |
| | ATOM | 1441 | N | MET | A | 490 | 31.387 | 8.274 | 9.058 | 1.00 | 31.33 |
| 35 | ATOM | 1442 | CA | MET | A | 490 | 31.056 | 9.482 | 9.801 | 1.00 | 30.61 |
| | ATOM | 1443 | CB | MET | A | 490 | 30.000 | 9.161 | 10.862 | 1.00 | 32.34 |
| | ATOM | 1444 | CG | MET | A | 490 | 28.607 | 8.940 | 10.289 | 1.00 | 30.71 |
| | ATOM | 1445 | SD | MET | A | 490 | 27.457 | 8.247 | 11.496 | 1.00 | 31.14 |
| | ATOM | 1446 | CE | MET | A | 490 | 26.321 | 7.408 | 10.418 | 1.00 | 30.36 |
| 40 | ATOM | 1447 | C | MET | A | 490 | 32.287 | 10.108 | 10.455 | 1.00 | 32.22 |
| | ATOM | 1448 | O | MET | A | 490 | 32.412 | 11.330 | 10.517 | 1.00 | 28.25 |
| | ATOM | 1449 | N | ALA | A | 491 | 33.184 | 9.262 | 10.949 | 1.00 | 33.81 |
| | ATOM | 1450 | CA | ALA | A | 491 | 34.407 | 9.730 | 11.585 | 1.00 | 39.92 |
| | ATOM | 1451 | CB | ALA | A | 491 | 35.168 | 8.554 | 12.185 | 1.00 | 37.22 |
| 45 | ATOM | 1452 | C | ALA | A | 491 | 35.275 | 10.445 | 10.550 | 1.00 | 42.68 |
| | ATOM | 1453 | O | ALA | A | 491 | 35.865 | 11.487 | 10.838 | 1.00 | 45.32 |
| | ATOM | 1454 | N | LYS | A | 492 | 35.339 | 9.876 | 9.347 | 1.00 | 44.39 |
| | ATOM | 1455 | CA | LYS | A | 492 | 36.122 | 10.440 | 8.248 | 1.00 | 44.80 |
| | ATOM | 1456 | CB | LYS | A | 492 | 36.136 | 9.477 | 7.052 | 1.00 | 46.96 |
| 50 | ATOM | 1457 | CG | LYS | A | 492 | 37.490 | 8.840 | 6.744 | 1.00 | 47.20 |
| | ATOM | 1458 | CD | LYS | A | 492 | 37.390 | 7.830 | 5.595 | 1.00 | 45.71 |
| | ATOM | 1459 | CE | LYS | A | 492 | 38.631 | 6.937 | 5.518 | 1.00 | 45.55 |
| | ATOM | 1460 | NZ | LYS | A | 492 | 38.357 | 5.577 | 4.948 | 1.00 | 36.28 |
| | ATOM | 1461 | C | LYS | A | 492 | 35.534 | 11.780 | 7.809 | 1.00 | 45.61 |
| 55 | ATOM | 1462 | O | LYS | A | 492 | 36.227 | 12.604 | 7.215 | 1.00 | 46.18 |
| | ATOM | 1463 | N | ALA | A | 493 | 34.254 | 11.992 | 8.100 | 1.00 | 43.75 |
| | ATOM | 1464 | CA | ALA | A | 493 | 33.590 | 13.238 | 7.728 | 1.00 | 42.42 |
| | ATOM | 1465 | CB | ALA | A | 493 | 32.097 | 13.001 | 7.528 | 1.00 | 40.92 |
| | ATOM | 1466 | C | ALA | A | 493 | 33.816 | 14.305 | 8.796 | 1.00 | 41.78 |
| 60 | ATOM | 1467 | O | ALA | A | 493 | 33.277 | 15.410 | 8.707 | 1.00 | 40.76 |
| | ATOM | 1468 | N | GLY | A | 494 | 34.604 | 13.960 | 9.811 | 1.00 | 41.01 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1469 | CA | GLY | A | 494 | 34.903 | 14.904 | 10.873 | 1.00 | 41.63 |
| | ATOM | 1470 | C | GLY | A | 494 | 33.857 | 15.060 | 11.965 | 1.00 | 41.18 |
| | ATOM | 1471 | O | GLY | A | 494 | 33.916 | 16.011 | 12.747 | 1.00 | 38.22 |
| | ATOM | 1472 | N | LEU | A | 495 | 32.905 | 14.138 | 12.043 | 1.00 | 39.53 |
| | ATOM | 1473 | CA | LEU | A | 495 | 31.876 | 14.248 | 13.068 | 1.00 | 38.91 |
| 10 | ATOM | 1474 | CB | LEU | A | 495 | 30.713 | 13.304 | 12.769 | 1.00 | 39.20 |
| | ATOM | 1475 | CG | LEU | A | 495 | 29.540 | 13.901 | 11.988 | 1.00 | 40.73 |
| | ATOM | 1476 | CD1 | LEU | A | 495 | 29.976 | 14.170 | 10.553 | 1.00 | 37.80 |
| | ATOM | 1477 | CD2 | LEU | A | 495 | 28.349 | 12.943 | 12.026 | 1.00 | 40.94 |
| | ATOM | 1478 | C | LEU | A | 495 | 32.461 | 13.923 | 14.431 | 1.00 | 36.01 |
| 15 | ATOM | 1479 | O | LEU | A | 495 | 33.347 | 13.074 | 14.544 | 1.00 | 34.85 |
| | ATOM | 1480 | N | THR | A | 496 | 31.979 | 14.604 | 15.459 | 1.00 | 37.52 |
| | ATOM | 1481 | CA | THR | A | 496 | 32.462 | 14.350 | 16.812 | 1.00 | 35.45 |
| | ATOM | 1482 | CB | THR | A | 496 | 31.925 | 15.375 | 17.829 | 1.00 | 37.55 |
| | ATOM | 1483 | OG1 | THR | A | 496 | 30.498 | 15.263 | 17.908 | 1.00 | 32.93 |
| 20 | ATOM | 1484 | CG2 | THR | A | 496 | 32.315 | 16.797 | 17.434 | 1.00 | 36.16 |
| | ATOM | 1485 | C | THR | A | 496 | 31.933 | 12.987 | 17.210 | 1.00 | 35.67 |
| | ATOM | 1486 | O | THR | A | 496 | 31.081 | 12.427 | 16.521 | 1.00 | 34.34 |
| | ATOM | 1487 | N | LEU | A | 497 | 32.429 | 12.452 | 18.319 | 1.00 | 34.88 |
| | ATOM | 1488 | CA | LEU | A | 497 | 31.965 | 11.151 | 18.786 | 1.00 | 35.67 |
| 25 | ATOM | 1489 | CB | LEU | A | 497 | 32.689 | 10.760 | 20.074 | 1.00 | 41.10 |
| | ATOM | 1490 | CG | LEU | A | 497 | 33.714 | 9.640 | 19.896 | 1.00 | 45.27 |
| | ATOM | 1491 | CD1 | LEU | A | 497 | 34.755 | 9.692 | 21.008 | 1.00 | 45.09 |
| | ATOM | 1492 | CD2 | LEU | A | 497 | 32.988 | 8.305 | 19.884 | 1.00 | 47.77 |
| | ATOM | 1493 | C | LEU | A | 497 | 30.455 | 11.198 | 19.026 | 1.00 | 33.72 |
| 30 | ATOM | 1494 | O | LEU | A | 497 | 29.712 | 10.350 | 18.534 | 1.00 | 33.20 |
| | ATOM | 1495 | N | GLN | A | 498 | 30.006 | 12.202 | 19.773 | 1.00 | 30.82 |
| | ATOM | 1496 | CA | GLN | A | 498 | 28.586 | 12.348 | 20.062 | 1.00 | 31.47 |
| | ATOM | 1497 | CB | GLN | A | 498 | 28.344 | 13.566 | 20.951 | 1.00 | 30.51 |
| | ATOM | 1498 | CG | GLN | A | 498 | 26.894 | 13.796 | 21.341 | 1.00 | 34.38 |
| 35 | ATOM | 1499 | CD | GLN | A | 498 | 26.712 | 15.130 | 22.015 | 1.00 | 38.60 |
| | ATOM | 1500 | OE1 | GLN | A | 498 | 27.363 | 16.112 | 21.686 | 1.00 | 42.92 |
| | ATOM | 1501 | NE2 | GLN | A | 498 | 25.809 | 15.176 | 23.008 | 1.00 | 40.02 |
| | ATOM | 1502 | C | GLN | A | 498 | 27.776 | 12.476 | 18.773 | 1.00 | 30.47 |
| | ATOM | 1503 | O | GLN | A | 498 | 26.682 | 11.927 | 18.665 | 1.00 | 30.85 |
| 40 | ATOM | 1504 | N | GLN | A | 499 | 28.311 | 13.196 | 17.793 | 1.00 | 29.52 |
| | ATOM | 1505 | CA | GLN | A | 499 | 27.603 | 13.362 | 16.524 | 1.00 | 30.24 |
| | ATOM | 1506 | CB | GLN | A | 499 | 28.292 | 14.420 | 15.661 | 1.00 | 30.20 |
| | ATOM | 1507 | CG | GLN | A | 499 | 28.135 | 15.840 | 16.191 | 1.00 | 31.60 |
| | ATOM | 1508 | CD | GLN | A | 499 | 28.930 | 16.849 | 15.389 | 1.00 | 31.61 |
| 45 | ATOM | 1509 | OE1 | GLN | A | 499 | 29.956 | 16.518 | 14.795 | 1.00 | 30.66 |
| | ATOM | 1510 | NE2 | GLN | A | 499 | 28.457 | 18.089 | 15.364 | 1.00 | 34.17 |
| | ATOM | 1511 | C | GLN | A | 499 | 27.529 | 12.047 | 15.753 | 1.00 | 29.40 |
| | ATOM | 1512 | O | GLN | A | 499 | 26.567 | 11.793 | 15.032 | 1.00 | 30.04 |
| | ATOM | 1513 | N | GLN | A | 500 | 28.550 | 11.214 | 15.903 | 1.00 | 25.67 |
| 50 | ATOM | 1514 | CA | GLN | A | 500 | 28.577 | 9.937 | 15.216 | 1.00 | 29.30 |
| | ATOM | 1515 | CB | GLN | A | 500 | 29.933 | 9.276 | 15.406 | 1.00 | 31.52 |
| | ATOM | 1516 | CG | GLN | A | 500 | 31.012 | 9.839 | 14.508 | 1.00 | 33.05 |
| | ATOM | 1517 | CD | GLN | A | 500 | 32.371 | 9.370 | 14.930 | 1.00 | 34.84 |
| | ATOM | 1518 | OE1 | GLN | A | 500 | 32.612 | 8.194 | 15.141 | 1.00 | 36.47 |
| 55 | ATOM | 1519 | NE2 | GLN | A | 500 | 33.301 | 10.324 | 15.082 | 1.00 | 38.25 |
| | ATOM | 1520 | C | GLN | A | 500 | 27.459 | 9.017 | 15.711 | 1.00 | 27.98 |
| | ATOM | 1521 | O | GLN | A | 500 | 26.700 | 8.469 | 14.908 | 1.00 | 24.84 |
| | ATOM | 1522 | N | HIS | A | 501 | 27.357 | 8.864 | 17.029 | 1.00 | 26.20 |
| | ATOM | 1523 | CA | HIS | A | 501 | 26.327 | 8.021 | 17.631 | 1.00 | 27.63 |
| 60 | ATOM | 1524 | CB | HIS | A | 501 | 26.535 | 7.919 | 19.145 | 1.00 | 27.97 |
| | ATOM | 1525 | CG | HIS | A | 501 | 27.892 | 7.420 | 19.535 | 1.00 | 34.27 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1526 | CD2 | HIS | A | 501 | 28.726 | 6.540 | 18.931 | 1.00 | 36.10 |
| | ATOM | 1527 | ND1 | HIS | A | 501 | 28.541 | 7.844 | 20.676 | 1.00 | 31.81 |
| | ATOM | 1528 | CE1 | HIS | A | 501 | 29.716 | 7.244 | 20.758 | 1.00 | 34.89 |
| | ATOM | 1529 | NE2 | HIS | A | 501 | 29.854 | 6.448 | 19.712 | 1.00 | 37.46 |
| | ATOM | 1530 | C | HIS | A | 501 | 24.935 | 8.572 | 17.348 | 1.00 | 24.93 |
| 10 | ATOM | 1531 | O | HIS | A | 501 | 23.998 | 7.815 | 17.107 | 1.00 | 26.73 |
| | ATOM | 1532 | N | GLN | A | 502 | 24.796 | 9.892 | 17.379 | 1.00 | 22.79 |
| | ATOM | 1533 | CA | GLN | A | 502 | 23.504 | 10.498 | 17.119 | 1.00 | 26.14 |
| | ATOM | 1534 | CB | GLN | A | 502 | 23.554 | 12.006 | 17.371 | 1.00 | 22.36 |
| | ATOM | 1535 | CG | GLN | A | 502 | 23.460 | 12.378 | 18.848 | 1.00 | 26.19 |
| 15 | ATOM | 1536 | CD | GLN | A | 502 | 23.589 | 13.875 | 19.089 | 1.00 | 28.67 |
| | ATOM | 1537 | OE1 | GLN | A | 502 | 23.632 | 14.663 | 18.149 | 1.00 | 28.40 |
| | ATOM | 1538 | NE2 | GLN | A | 502 | 23.651 | 14.268 | 20.355 | 1.00 | 24.72 |
| | ATOM | 1539 | C | GLN | A | 502 | 23.056 | 10.221 | 15.685 | 1.00 | 26.19 |
| | ATOM | 1540 | O | GLN | A | 502 | 21.913 | 9.822 | 15.453 | 1.00 | 24.09 |
| 20 | ATOM | 1541 | N | ARG | A | 503 | 23.955 | 10.429 | 14.727 | 1.00 | 24.88 |
| | ATOM | 1542 | CA | ARG | A | 503 | 23.630 | 10.196 | 13.326 | 1.00 | 25.25 |
| | ATOM | 1543 | CB | ARG | A | 503 | 24.772 | 10.668 | 12.418 | 1.00 | 27.63 |
| | ATOM | 1544 | CG | ARG | A | 503 | 24.432 | 10.563 | 10.932 | 1.00 | 28.75 |
| | ATOM | 1545 | CD | ARG | A | 503 | 25.479 | 11.222 | 10.056 | 1.00 | 27.72 |
| 25 | ATOM | 1546 | NE | ARG | A | 503 | 25.072 | 11.214 | 8.654 | 1.00 | 29.35 |
| | ATOM | 1547 | CZ | ARG | A | 503 | 24.279 | 12.126 | 8.105 | 1.00 | 25.84 |
| | ATOM | 1548 | NH1 | ARG | A | 503 | 23.804 | 13.120 | 8.840 | 1.00 | 27.35 |
| | ATOM | 1549 | NH2 | ARG | A | 503 | 23.962 | 12.044 | 6.820 | 1.00 | 30.63 |
| | ATOM | 1550 | C | ARG | A | 503 | 23.347 | 8.716 | 13.065 | 1.00 | 24.53 |
| 30 | ATOM | 1551 | O | ARG | A | 503 | 22.425 | 8.375 | 12.321 | 1.00 | 25.90 |
| | ATOM | 1552 | N | LEU | A | 504 | 24.143 | 7.841 | 13.672 | 1.00 | 23.00 |
| | ATOM | 1553 | CA | LEU | A | 504 | 23.953 | 6.406 | 13.496 | 1.00 | 22.60 |
| | ATOM | 1554 | CB | LEU | A | 504 | 24.971 | 5.621 | 14.323 | 1.00 | 25.43 |
| | ATOM | 1555 | CG | LEU | A | 504 | 24.781 | 4.100 | 14.344 | 1.00 | 25.23 |
| 35 | ATOM | 1556 | CD1 | LEU | A | 504 | 25.166 | 3.505 | 12.991 | 1.00 | 28.52 |
| | ATOM | 1557 | CD2 | LEU | A | 504 | 25.627 | 3.495 | 15.444 | 1.00 | 22.14 |
| | ATOM | 1558 | C | LEU | A | 504 | 22.541 | 6.030 | 13.934 | 1.00 | 22.84 |
| | ATOM | 1559 | O | LEU | A | 504 | 21.846 | 5.288 | 13.245 | 1.00 | 21.51 |
| | ATOM | 1560 | N | ALA | A | 505 | 22.120 | 6.547 | 15.083 | 1.00 | 20.16 |
| 40 | ATOM | 1561 | CA | ALA | A | 505 | 20.784 | 6.262 | 15.585 | 1.00 | 21.08 |
| | ATOM | 1562 | CB | ALA | A | 505 | 20.605 | 6.868 | 16.980 | 1.00 | 23.57 |
| | ATOM | 1563 | C | ALA | A | 505 | 19.738 | 6.832 | 14.628 | 1.00 | 20.20 |
| | ATOM | 1564 | O | ALA | A | 505 | 18.754 | 6.164 | 14.293 | 1.00 | 17.31 |
| | ATOM | 1565 | N | GLN | A | 506 | 19.954 | 8.066 | 14.184 | 1.00 | 22.11 |
| 45 | ATOM | 1566 | CA | GLN | A | 506 | 19.013 | 8.711 | 13.277 | 1.00 | 21.70 |
| | ATOM | 1567 | CB | GLN | A | 506 | 19.502 | 10.111 | 12.903 | 1.00 | 22.26 |
| | ATOM | 1568 | CG | GLN | A | 506 | 19.240 | 11.158 | 13.975 | 1.00 | 25.84 |
| | ATOM | 1569 | CD | GLN | A | 506 | 20.187 | 12.333 | 13.857 | 1.00 | 32.88 |
| | ATOM | 1570 | OE1 | GLN | A | 506 | 20.704 | 12.614 | 12.777 | 1.00 | 31.23 |
| 50 | ATOM | 1571 | NE2 | GLN | A | 506 | 20.423 | 13.025 | 14.968 | 1.00 | 32.97 |
| | ATOM | 1572 | C | GLN | A | 506 | 18.813 | 7.881 | 12.016 | 1.00 | 23.57 |
| | ATOM | 1573 | O | GLN | A | 506 | 17.684 | 7.715 | 11.550 | 1.00 | 21.83 |
| | ATOM | 1574 | N | LEU | A | 507 | 19.905 | 7.354 | 11.474 | 1.00 | 19.98 |
| | ATOM | 1575 | CA | LEU | A | 507 | 19.827 | 6.537 | 10.263 | 1.00 | 22.03 |
| 55 | ATOM | 1576 | CB | LEU | A | 507 | 21.231 | 6.244 | 9.725 | 1.00 | 23.02 |
| | ATOM | 1577 | CG | LEU | A | 507 | 22.026 | 7.457 | 9.225 | 1.00 | 25.80 |
| | ATOM | 1578 | CD1 | LEU | A | 507 | 23.371 | 6.994 | 8.713 | 1.00 | 27.67 |
| | ATOM | 1579 | CD2 | LEU | A | 507 | 21.264 | 8.176 | 8.130 | 1.00 | 25.62 |
| | ATOM | 1580 | C | LEU | A | 507 | 19.090 | 5.219 | 10.496 | 1.00 | 22.35 |
| 60 | ATOM | 1581 | O | LEU | A | 507 | 18.242 | 4.825 | 9.695 | 1.00 | 19.33 |
| | ATOM | 1582 | N | LEU | A | 508 | 19.402 | 4.539 | 11.592 | 1.00 | 21.29 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1583 | CA | LEU | A | 508 | 18.755 | 3.260 | 11.881 | 1.00 | 20.72 |
| | ATOM | 1584 | CB | LEU | A | 508 | 19.501 | 2.535 | 13.001 | 1.00 | 22.29 |
| | ATOM | 1585 | CG | LEU | A | 508 | 20.977 | 2.311 | 12.678 | 1.00 | 24.70 |
| | ATOM | 1586 | CD1 | LEU | A | 508 | 21.642 | 1.551 | 13.814 | 1.00 | 21.37 |
| | ATOM | 1587 | CD2 | LEU | A | 508 | 21.095 | 1.542 | 11.367 | 1.00 | 27.88 |
| 10 | ATOM | 1588 | C | LEU | A | 508 | 17.279 | 3.396 | 12.239 | 1.00 | 19.14 |
| | ATOM | 1589 | O | LEU | A | 508 | 16.498 | 2.478 | 12.003 | 1.00 | 17.80 |
| | ATOM | 1590 | N | LEU | A | 509 | 16.895 | 4.530 | 12.815 | 1.00 | 19.23 |
| | ATOM | 1591 | CA | LEU | A | 509 | 15.495 | 4.747 | 13.173 | 1.00 | 20.14 |
| | ATOM | 1592 | CB | LEU | A | 509 | 15.347 | 6.030 | 13.999 | 1.00 | 20.28 |
| 15 | ATOM | 1593 | CG | LEU | A | 509 | 15.710 | 5.858 | 15.479 | 1.00 | 21.35 |
| | ATOM | 1594 | CD1 | LEU | A | 509 | 15.354 | 7.106 | 16.263 | 1.00 | 19.29 |
| | ATOM | 1595 | CD2 | LEU | A | 509 | 14.989 | 4.656 | 16.038 | 1.00 | 20.84 |
| | ATOM | 1596 | C | LEU | A | 509 | 14.681 | 4.841 | 11.885 | 1.00 | 21.69 |
| | ATOM | 1597 | O | LEU | A | 509 | 13.493 | 4.514 | 11.854 | 1.00 | 22.40 |
| 20 | ATOM | 1598 | N | ILE | A | 510 | 15.343 | 5.270 | 10.815 | 1.00 | 20.22 |
| | ATOM | 1599 | CA | ILE | A | 510 | 14.710 | 5.397 | 9.508 | 1.00 | 20.40 |
| | ATOM | 1600 | CB | ILE | A | 510 | 15.720 | 5.946 | 8.464 | 1.00 | 28.34 |
| | ATOM | 1601 | CG2 | ILE | A | 510 | 15.208 | 5.710 | 7.056 | 1.00 | 32.54 |
| | ATOM | 1602 | CG1 | ILE | A | 510 | 15.965 | 7.438 | 8.696 | 1.00 | 28.23 |
| 25 | ATOM | 1603 | CD1 | ILE | A | 510 | 14.789 | 8.189 | 9.288 | 1.00 | 33.16 |
| | ATOM | 1604 | C | ILE | A | 510 | 14.210 | 4.025 | 9.049 | 1.00 | 23.21 |
| | ATOM | 1605 | O | ILE | A | 510 | 13.120 | 3.906 | 8.474 | 1.00 | 21.16 |
| | ATOM | 1606 | N | LEU | A | 511 | 14.998 | 2.989 | 9.323 | 1.00 | 18.38 |
| | ATOM | 1607 | CA | LEU | A | 511 | 14.633 | 1.634 | 8.917 | 1.00 | 20.10 |
| 30 | ATOM | 1608 | CB | LEU | A | 511 | 15.754 | 0.656 | 9.267 | 1.00 | 21.69 |
| | ATOM | 1609 | CG | LEU | A | 511 | 17.128 | 1.022 | 8.692 | 1.00 | 26.03 |
| | ATOM | 1610 | CD1 | LEU | A | 511 | 18.024 | -0.206 | 8.724 | 1.00 | 22.68 |
| | ATOM | 1611 | CD2 | LEU | A | 511 | 16.996 | 1.544 | 7.267 | 1.00 | 26.00 |
| | ATOM | 1612 | C | LEU | A | 511 | 13.326 | 1.181 | 9.543 | 1.00 | 18.51 |
| 35 | ATOM | 1613 | O | LEU | A | 511 | 12.663 | 0.283 | 9.025 | 1.00 | 17.40 |
| | ATOM | 1614 | N | SER | A | 512 | 12.963 | 1.799 | 10.664 | 1.00 | 18.68 |
| | ATOM | 1615 | CA | SER | A | 512 | 11.718 | 1.471 | 11.331 | 1.00 | 18.67 |
| | ATOM | 1616 | CB | SER | A | 512 | 11.661 | 2.117 | 12.720 | 1.00 | 18.58 |
| | ATOM | 1617 | OG | SER | A | 512 | 10.315 | 2.229 | 13.165 | 1.00 | 27.92 |
| 40 | ATOM | 1618 | C | SER | A | 512 | 10.572 | 1.994 | 10.464 | 1.00 | 18.43 |
| | ATOM | 1619 | O | SER | A | 512 | 9.584 | 1.296 | 10.236 | 1.00 | 13.91 |
| | ATOM | 1620 | N | HIS | A | 513 | 10.713 | 3.228 | 9.982 | 1.00 | 18.95 |
| | ATOM | 1621 | CA | HIS | A | 513 | 9.698 | 3.831 | 9.124 | 1.00 | 20.82 |
| | ATOM | 1622 | CB | HIS | A | 513 | 10.013 | 5.315 | 8.894 | 1.00 | 24.36 |
| 45 | ATOM | 1623 | CG | HIS | A | 513 | 9.923 | 6.146 | 10.136 | 1.00 | 32.13 |
| | ATOM | 1624 | CD2 | HIS | A | 513 | 8.863 | 6.744 | 10.734 | 1.00 | 35.29 |
| | ATOM | 1625 | ND1 | HIS | A | 513 | 11.010 | 6.391 | 10.949 | 1.00 | 35.00 |
| | ATOM | 1626 | CE1 | HIS | A | 513 | 10.624 | 7.101 | 11.995 | 1.00 | 34.67 |
| | ATOM | 1627 | NE2 | HIS | A | 513 | 9.326 | 7.328 | 11.889 | 1.00 | 35.82 |
| 50 | ATOM | 1628 | C | HIS | A | 513 | 9.650 | 3.079 | 7.790 | 1.00 | 19.08 |
| | ATOM | 1629 | O | HIS | A | 513 | 8.575 | 2.863 | 7.220 | 1.00 | 21.20 |
| | ATOM | 1630 | N | ILE | A | 514 | 10.809 | 2.662 | 7.297 | 1.00 | 15.58 |
| | ATOM | 1631 | CA | ILE | A | 514 | 10.849 | 1.921 | 6.038 | 1.00 | 16.48 |
| | ATOM | 1632 | CB | ILE | A | 514 | 12.312 | 1.678 | 5.576 | 1.00 | 20.09 |
| 55 | ATOM | 1633 | CG2 | ILE | A | 514 | 12.349 | 0.602 | 4.499 | 1.00 | 19.55 |
| | ATOM | 1634 | CG1 | ILE | A | 514 | 12.891 | 2.986 | 5.019 | 1.00 | 22.62 |
| | ATOM | 1635 | CD1 | ILE | A | 514 | 14.393 | 2.992 | 4.874 | 1.00 | 27.34 |
| | ATOM | 1636 | C | ILE | A | 514 | 10.112 | 0.590 | 6.210 | 1.00 | 16.40 |
| | ATOM | 1637 | O | ILE | A | 514 | 9.364 | 0.164 | 5.328 | 1.00 | 17.91 |
| 60 | ATOM | 1638 | N | ARG | A | 515 | 10.301 | -0.071 | 7.347 | 1.00 | 18.20 |
| | ATOM | 1639 | CA | ARG | A | 515 | 9.585 | -1.327 | 7.564 | 1.00 | 18.05 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1640 | CB | ARG | A | 515 | 9.984 | -1.980 | 8.889 | 1.00 | 18.36 |
| | ATOM | 1641 | CG | ARG | A | 515 | 9.173 | -3.237 | 9.213 | 1.00 | 17.84 |
| | ATOM | 1642 | CD | ARG | A | 515 | 9.823 | -4.470 | 8.606 | 1.00 | 17.94 |
| | ATOM | 1643 | NE | ARG | A | 515 | 11.038 | -4.813 | 9.334 | 1.00 | 26.96 |
| | ATOM | 1644 | CZ | ARG | A | 515 | 11.406 | -6.051 | 9.641 | 1.00 | 25.13 |
| 10 | ATOM | 1645 | NH1 | ARG | A | 515 | 10.654 | -7.080 | 9.281 | 1.00 | 23.49 |
| | ATOM | 1646 | NH2 | ARG | A | 515 | 12.511 | -6.254 | 10.340 | 1.00 | 32.16 |
| | ATOM | 1647 | C | ARG | A | 515 | 8.089 | -1.020 | 7.594 | 1.00 | 18.29 |
| | ATOM | 1648 | O | ARG | A | 515 | 7.275 | -1.759 | 7.038 | 1.00 | 16.22 |
| | ATOM | 1649 | N | HIS | A | 516 | 7.726 | 0.085 | 8.237 | 1.00 | 19.33 |
| 15 | ATOM | 1650 | CA | HIS | A | 516 | 6.317 | 0.441 | 8.330 | 1.00 | 17.78 |
| | ATOM | 1651 | CB | HIS | A | 516 | 6.126 | 1.702 | 9.166 | 1.00 | 16.84 |
| | ATOM | 1652 | CG | HIS | A | 516 | 4.692 | 2.101 | 9.312 | 1.00 | 18.16 |
| | ATOM | 1653 | CD2 | HIS | A | 516 | 3.967 | 3.061 | 8.691 | 1.00 | 21.17 |
| | ATOM | 1654 | ND1 | HIS | A | 516 | 3.830 | 1.469 | 10.180 | 1.00 | 20.70 |
| 20 | ATOM | 1655 | CE1 | HIS | A | 516 | 2.633 | 2.022 | 10.089 | 1.00 | 21.52 |
| | ATOM | 1656 | NE2 | HIS | A | 516 | 2.689 | 2.992 | 9.191 | 1.00 | 20.16 |
| | ATOM | 1657 | C | HIS | A | 516 | 5.708 | 0.659 | 6.954 | 1.00 | 16.63 |
| | ATOM | 1658 | O | HIS | A | 516 | 4.598 | 0.216 | 6.689 | 1.00 | 18.58 |
| | ATOM | 1659 | N | MET | A | 517 | 6.438 | 1.334 | 6.073 | 1.00 | 15.29 |
| 25 | ATOM | 1660 | CA | MET | A | 517 | 5.925 | 1.589 | 4.730 | 1.00 | 16.58 |
| | ATOM | 1661 | CB | MET | A | 517 | 6.837 | 2.576 | 4.002 | 1.00 | 18.66 |
| | ATOM | 1662 | CG | MET | A | 517 | 6.805 | 3.978 | 4.631 | 1.00 | 16.88 |
| | ATOM | 1663 | SD | MET | A | 517 | 7.670 | 5.243 | 3.701 | 1.00 | 24.08 |
| | ATOM | 1664 | CE | MET | A | 517 | 9.390 | 4.777 | 3.962 | 1.00 | 14.30 |
| 30 | ATOM | 1665 | C | MET | A | 517 | 5.773 | 0.289 | 3.940 | 1.00 | 17.86 |
| | ATOM | 1666 | O | MET | A | 517 | 4.791 | 0.101 | 3.224 | 1.00 | 18.25 |
| | ATOM | 1667 | N | SER | A | 518 | 6.741 | -0.610 | 4.086 | 1.00 | 17.43 |
| | ATOM | 1668 | CA | SER | A | 518 | 6.697 | -1.896 | 3.403 | 1.00 | 18.40 |
| | ATOM | 1669 | CB | SER | A | 518 | 7.974 | -2.695 | 3.680 | 1.00 | 16.77 |
| 35 | ATOM | 1670 | OG | SER | A | 518 | 7.834 | -4.030 | 3.227 | 1.00 | 24.23 |
| | ATOM | 1671 | C | SER | A | 518 | 5.476 | -2.695 | 3.854 | 1.00 | 17.91 |
| | ATOM | 1672 | O | SER | A | 518 | 4.788 | -3.295 | 3.030 | 1.00 | 18.97 |
| | ATOM | 1673 | N | ASN | A | 519 | 5.204 | -2.697 | 5.159 | 1.00 | 21.82 |
| | ATOM | 1674 | CA | ASN | A | 519 | 4.047 | -3.418 | 5.696 | 1.00 | 21.99 |
| 40 | ATOM | 1675 | CB | ASN | A | 519 | 3.957 | -3.257 | 7.216 | 1.00 | 23.24 |
| | ATOM | 1676 | CG | ASN | A | 519 | 5.046 | -4.011 | 7.957 | 1.00 | 31.14 |
| | ATOM | 1677 | OD1 | ASN | A | 519 | 5.585 | -4.999 | 7.461 | 1.00 | 32.50 |
| | ATOM | 1678 | ND2 | ASN | A | 519 | 5.368 | -3.545 | 9.163 | 1.00 | 29.10 |
| | ATOM | 1679 | C | ASN | A | 519 | 2.761 | -2.871 | 5.079 | 1.00 | 23.76 |
| 45 | ATOM | 1680 | O | ASN | A | 519 | 1.902 | -3.632 | 4.631 | 1.00 | 24.48 |
| | ATOM | 1681 | N | LYS | A | 520 | 2.627 | -1.548 | 5.078 | 1.00 | 20.58 |
| | ATOM | 1682 | CA | LYS | A | 520 | 1.449 | -0.900 | 4.512 | 1.00 | 25.49 |
| | ATOM | 1683 | CB | LYS | A | 520 | 1.484 | 0.607 | 4.786 | 1.00 | 24.73 |
| | ATOM | 1684 | CG | LYS | A | 520 | 1.512 | 0.996 | 6.264 | 1.00 | 32.31 |
| 50 | ATOM | 1685 | CD | LYS | A | 520 | 0.656 | 0.080 | 7.133 | 1.00 | 37.11 |
| | ATOM | 1686 | CE | LYS | A | 520 | -0.787 | 0.547 | 7.181 | 1.00 | 41.56 |
| | ATOM | 1687 | NZ | LYS | A | 520 | -1.560 | -0.134 | 8.261 | 1.00 | 42.66 |
| | ATOM | 1688 | C | LYS | A | 520 | 1.380 | -1.144 | 3.005 | 1.00 | 25.40 |
| | ATOM | 1689 | O | LYS | A | 520 | 0.316 | -1.436 | 2.467 | 1.00 | 26.44 |
| 55 | ATOM | 1690 | N | GLY | A | 521 | 2.520 | -1.021 | 2.332 | 1.00 | 22.88 |
| | ATOM | 1691 | CA | GLY | A | 521 | 2.561 | -1.236 | 0.897 | 1.00 | 21.53 |
| | ATOM | 1692 | C | GLY | A | 521 | 2.177 | -2.655 | 0.536 | 1.00 | 24.79 |
| | ATOM | 1693 | O | GLY | A | 521 | 1.426 | -2.878 | -0.413 | 1.00 | 25.71 |
| | ATOM | 1694 | N | MET | A | 522 | 2.696 | -3.619 | 1.290 | 1.00 | 22.75 |
| 60 | ATOM | 1695 | CA | MET | A | 522 | 2.393 | -5.027 | 1.058 | 1.00 | 23.40 |
| | ATOM | 1696 | CB | MET | A | 522 | 3.170 | -5.898 | 2.042 | 1.00 | 25.74 |

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 1697 | CG | MET | A | 522 | 3.396 | -7.308 | 1.559 | 1.00 | 31.06 |
| | ATOM | 1698 | SD | MET | A | 522 | 4.572 | -7.352 | 0.202 | 1.00 | 34.06 |
| | ATOM | 1699 | CE | MET | A | 522 | 6.125 | -7.229 | 1.113 | 1.00 | 29.28 |
| | ATOM | 1700 | C | MET | A | 522 | 0.893 | -5.281 | 1.218 | 1.00 | 26.49 |
| | ATOM | 1701 | O | MET | A | 522 | 0.268 | -5.920 | 0.361 | 1.00 | 25.47 |
| 10 | ATOM | 1702 | N | GLU | A | 523 | 0.321 | -4.790 | 2.318 | 1.00 | 24.95 |
| | ATOM | 1703 | CA | GLU | A | 523 | -1.110 | -4.954 | 2.566 | 1.00 | 27.15 |
| | ATOM | 1704 | CB | GLU | A | 523 | -1.555 | -4.206 | 3.835 | 1.00 | 31.08 |
| | ATOM | 1705 | CG | GLU | A | 523 | -0.830 | -4.564 | 5.124 | 1.00 | 38.93 |
| | ATOM | 1706 | CD | GLU | A | 523 | -1.153 | -3.585 | 6.258 | 1.00 | 46.90 |
| 15 | ATOM | 1707 | OE1 | GLU | A | 523 | -2.225 | -2.938 | 6.200 | 1.00 | 47.40 |
| | ATOM | 1708 | OE2 | GLU | A | 523 | -0.337 | -3.460 | 7.202 | 1.00 | 47.39 |
| | ATOM | 1709 | C | GLU | A | 523 | -1.872 | -4.368 | 1.381 | 1.00 | 26.10 |
| | ATOM | 1710 | O | GLU | A | 523 | -2.817 | -4.964 | 0.882 | 1.00 | 24.25 |
| | ATOM | 1711 | N | HIS | A | 524 | -1.449 | -3.182 | 0.940 | 1.00 | 24.74 |
| 20 | ATOM | 1712 | CA | HIS | A | 524 | -2.093 | -2.505 | -0.173 | 1.00 | 26.17 |
| | ATOM | 1713 | CB | HIS | A | 524 | -1.481 | -1.125 | -0.379 | 1.00 | 24.64 |
| | ATOM | 1714 | CG | HIS | A | 524 | -2.233 | -0.278 | -1.355 | 1.00 | 30.59 |
| | ATOM | 1715 | CD2 | HIS | A | 524 | -3.227 | 0.624 | -1.172 | 1.00 | 32.15 |
| | ATOM | 1716 | ND1 | HIS | A | 524 | -2.008 | -0.332 | -2.713 | 1.00 | 27.46 |
| 25 | ATOM | 1717 | CE1 | HIS | A | 524 | -2.829 | 0.502 | -3.326 | 1.00 | 34.58 |
| | ATOM | 1718 | NE2 | HIS | A | 524 | -3.580 | 1.094 | -2.413 | 1.00 | 30.50 |
| | ATOM | 1719 | C | HIS | A | 524 | -1.996 | -3.294 | -1.474 | 1.00 | 28.06 |
| | ATOM | 1720 | O | HIS | A | 524 | -2.976 | -3.419 | -2.217 | 1.00 | 29.81 |
| | ATOM | 1721 | N | LEU | A | 525 | -0.811 | -3.824 | -1.746 | 1.00 | 27.07 |
| 30 | ATOM | 1722 | CA | LEU | A | 525 | -0.594 | -4.601 | -2.955 | 1.00 | 29.30 |
| | ATOM | 1723 | CB | LEU | A | 525 | 0.865 | -5.039 | -3.051 | 1.00 | 26.39 |
| | ATOM | 1724 | CG | LEU | A | 525 | 1.307 | -5.765 | -4.321 | 1.00 | 29.34 |
| | ATOM | 1725 | CD1 | LEU | A | 525 | 0.734 | -5.076 | -5.562 | 1.00 | 29.61 |
| | ATOM | 1726 | CD2 | LEU | A | 525 | 2.829 | -5.769 | -4.370 | 1.00 | 29.22 |
| 35 | ATOM | 1727 | C | LEU | A | 525 | -1.497 | -5.822 | -2.950 | 1.00 | 31.67 |
| | ATOM | 1728 | O | LEU | A | 525 | -2.128 | -6.133 | -3.957 | 1.00 | 32.45 |
| | ATOM | 1729 | N | TYR | A | 526 | -1.559 | -6.512 | -1.814 | 1.00 | 36.14 |
| | ATOM | 1730 | CA | TYR | A | 526 | -2.397 | -7.698 | -1.696 | 1.00 | 40.36 |
| | ATOM | 1731 | CB | TYR | A | 526 | -2.221 | -8.350 | -0.324 | 1.00 | 45.27 |
| 40 | ATOM | 1732 | CG | TYR | A | 526 | -2.849 | -9.722 | -0.229 | 1.00 | 50.62 |
| | ATOM | 1733 | CD1 | TYR | A | 526 | -2.114 | -10.867 | -0.537 | 1.00 | 54.55 |
| | ATOM | 1734 | CE1 | TYR | A | 526 | -2.698 | -12.136 | -0.482 | 1.00 | 57.27 |
| | ATOM | 1735 | CD2 | TYR | A | 526 | -4.188 | -9.876 | 0.142 | 1.00 | 53.48 |
| | ATOM | 1736 | CE2 | TYR | A | 526 | -4.781 | -11.141 | 0.201 | 1.00 | 55.93 |
| 45 | ATOM | 1737 | CZ | TYR | A | 526 | -4.029 | -12.264 | -0.113 | 1.00 | 56.60 |
| | ATOM | 1738 | OH | TYR | A | 526 | -4.603 | -13.515 | -0.063 | 1.00 | 60.70 |
| | ATOM | 1739 | C | TYR | A | 526 | -3.852 | -7.298 | -1.893 | 1.00 | 42.83 |
| | ATOM | 1740 | O | TYR | A | 526 | -4.673 | -8.094 | -2.349 | 1.00 | 43.49 |
| | ATOM | 1741 | N | SER | A | 527 | -4.158 | -6.055 | -1.543 | 1.00 | 41.55 |
| 50 | ATOM | 1742 | CA | SER | A | 527 | -5.503 | -5.523 | -1.686 | 1.00 | 44.04 |
| | ATOM | 1743 | CB | SER | A | 527 | -5.606 | -4.169 | -0.979 | 1.00 | 43.47 |
| | ATOM | 1744 | OG | SER | A | 527 | -6.954 | -3.789 | -0.786 | 1.00 | 47.51 |
| | ATOM | 1745 | C | SER | A | 527 | -5.817 | -5.356 | -3.172 | 1.00 | 44.18 |
| | ATOM | 1746 | O | SER | A | 527 | -6.883 | -5.757 | -3.642 | 1.00 | 44.88 |
| 55 | ATOM | 1747 | N | MET | A | 528 | -4.883 | -4.755 | -3.901 | 1.00 | 41.79 |
| | ATOM | 1748 | CA | MET | A | 528 | -5.047 | -4.536 | -5.331 | 1.00 | 44.04 |
| | ATOM | 1749 | CB | MET | A | 528 | -3.898 | -3.679 | -5.870 | 1.00 | 44.78 |
| | ATOM | 1750 | CG | MET | A | 528 | -3.965 | -2.206 | -5.468 | 1.00 | 45.37 |
| | ATOM | 1751 | SD | MET | A | 528 | -5.652 | -1.598 | -5.273 | 1.00 | 51.83 |
| 60 | ATOM | 1752 | CE | MET | A | 528 | -5.553 | -0.004 | -6.044 | 1.00 | 46.61 |
| | ATOM | 1753 | C | MET | A | 528 | -5.087 | -5.871 | -6.071 | 1.00 | 44.29 |

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|----|------|------|-----|-----|---|-----|--------|---------|---------|------|-------|
| 5 | ATOM | 1754 | O | MET | A | 528 | -5.689 | -5.979 | -7.137 | 1.00 | 44.02 |
| | ATOM | 1755 | N | LYS | A | 529 | -4.443 | -6.883 | -5.499 | 1.00 | 46.78 |
| | ATOM | 1756 | CA | LYS | A | 529 | -4.413 | -8.213 | -6.099 | 1.00 | 51.28 |
| | ATOM | 1757 | CB | LYS | A | 529 | -3.550 | -9.158 | -5.261 | 1.00 | 50.87 |
| | ATOM | 1758 | CG | LYS | A | 529 | -2.798 | -10.204 | -6.071 | 1.00 | 50.55 |
| 10 | ATOM | 1759 | CD | LYS | A | 529 | -3.548 | -11.520 | -6.104 | 1.00 | 51.25 |
| | ATOM | 1760 | CE | LYS | A | 529 | -2.616 | -12.694 | -5.856 | 1.00 | 53.22 |
| | ATOM | 1761 | NZ | LYS | A | 529 | -2.420 | -12.954 | -4.402 | 1.00 | 53.22 |
| | ATOM | 1762 | C | LYS | A | 529 | -5.829 | -8.768 | -6.182 | 1.00 | 54.27 |
| | ATOM | 1763 | O | LYS | A | 529 | -6.325 | -9.069 | -7.266 | 1.00 | 55.50 |
| 15 | ATOM | 1764 | N | CYS | A | 530 | -6.472 | -8.901 | -5.027 | 1.00 | 56.71 |
| | ATOM | 1765 | CA | CYS | A | 530 | -7.833 | -9.416 | -4.961 | 1.00 | 58.35 |
| | ATOM | 1766 | CB | CYS | A | 530 | -8.333 | -9.380 | -3.517 | 1.00 | 59.78 |
| | ATOM | 1767 | SG | CYS | A | 530 | -7.289 | -10.304 | -2.358 | 1.00 | 63.19 |
| | ATOM | 1768 | C | CYS | A | 530 | -8.766 | -8.609 | -5.858 | 1.00 | 59.36 |
| 20 | ATOM | 1769 | O | CYS | A | 530 | -9.644 | -9.169 | -6.514 | 1.00 | 59.52 |
| | ATOM | 1770 | N | LYS | A | 531 | -8.569 | -7.293 | -5.888 | 1.00 | 59.24 |
| | ATOM | 1771 | CA | LYS | A | 531 | -9.390 | -6.411 | -6.713 | 1.00 | 60.14 |
| | ATOM | 1772 | CB | LYS | A | 531 | -9.158 | -4.952 | -6.317 | 1.00 | 58.92 |
| | ATOM | 1773 | C | LYS | A | 531 | -9.073 | -6.615 | -8.195 | 1.00 | 61.48 |
| 25 | ATOM | 1774 | O | LYS | A | 531 | -9.618 | -5.928 | -9.061 | 1.00 | 61.74 |
| | ATOM | 1775 | N | ASN | A | 532 | -8.179 | -7.561 | -8.474 | 1.00 | 61.65 |
| | ATOM | 1776 | CA | ASN | A | 532 | -7.783 | -7.890 | -9.840 | 1.00 | 61.60 |
| | ATOM | 1777 | CB | ASN | A | 532 | -8.966 | -8.518 | -10.581 | 1.00 | 62.28 |
| | ATOM | 1778 | CG | ASN | A | 532 | -8.750 | -9.985 | -10.878 | 1.00 | 64.66 |
| 30 | ATOM | 1779 | OD1 | ASN | A | 532 | -8.344 | -10.352 | -11.983 | 1.00 | 67.08 |
| | ATOM | 1780 | ND2 | ASN | A | 532 | -9.016 | -10.836 | -9.891 | 1.00 | 62.68 |
| | ATOM | 1781 | C | ASN | A | 532 | -7.247 | -6.710 | -10.648 | 1.00 | 59.75 |
| | ATOM | 1782 | O | ASN | A | 532 | -7.487 | -6.615 | -11.850 | 1.00 | 57.50 |
| | ATOM | 1783 | N | VAL | A | 533 | -6.507 | -5.822 | -9.992 | 1.00 | 59.39 |
| 35 | ATOM | 1784 | CA | VAL | A | 533 | -5.954 | -4.656 | -10.669 | 1.00 | 58.22 |
| | ATOM | 1785 | CB | VAL | A | 533 | -6.223 | -3.371 | -9.865 | 1.00 | 59.20 |
| | ATOM | 1786 | CG1 | VAL | A | 533 | -6.181 | -2.163 | -10.785 | 1.00 | 59.21 |
| | ATOM | 1787 | CG2 | VAL | A | 533 | -7.574 | -3.467 | -9.172 | 1.00 | 59.57 |
| | ATOM | 1788 | C | VAL | A | 533 | -4.452 | -4.767 | -10.907 | 1.00 | 57.86 |
| 40 | ATOM | 1789 | O | VAL | A | 533 | -3.846 | -3.874 | -11.499 | 1.00 | 60.56 |
| | ATOM | 1790 | N | VAL | A | 534 | -3.852 | -5.863 | -10.451 | 1.00 | 56.03 |
| | ATOM | 1791 | CA | VAL | A | 534 | -2.417 | -6.063 | -10.621 | 1.00 | 54.11 |
| | ATOM | 1792 | CB | VAL | A | 534 | -1.767 | -6.632 | -9.341 | 1.00 | 54.02 |
| | ATOM | 1793 | CG1 | VAL | A | 534 | -0.300 | -6.950 | -9.601 | 1.00 | 52.37 |
| 45 | ATOM | 1794 | CG2 | VAL | A | 534 | -1.900 | -5.635 | -8.200 | 1.00 | 55.70 |
| | ATOM | 1795 | C | VAL | A | 534 | -2.089 | -7.008 | -11.770 | 1.00 | 54.31 |
| | ATOM | 1796 | O | VAL | A | 534 | -2.519 | -8.164 | -11.780 | 1.00 | 51.66 |
| | ATOM | 1797 | N | PRO | A | 535 | -1.315 | -6.527 | -12.755 | 1.00 | 53.54 |
| | ATOM | 1798 | CD | PRO | A | 535 | -0.749 | -5.172 | -12.874 | 1.00 | 54.28 |
| 50 | ATOM | 1799 | CA | PRO | A | 535 | -0.949 | -7.373 | -13.893 | 1.00 | 53.24 |
| | ATOM | 1800 | CB | PRO | A | 535 | 0.011 | -6.500 | -14.697 | 1.00 | 52.71 |
| | ATOM | 1801 | CG | PRO | A | 535 | -0.353 | -5.102 | -14.319 | 1.00 | 53.19 |
| | ATOM | 1802 | C | PRO | A | 535 | -0.296 | -8.664 | -13.411 | 1.00 | 54.25 |
| | ATOM | 1803 | O | PRO | A | 535 | 0.121 | -8.768 | -12.254 | 1.00 | 54.56 |
| 55 | ATOM | 1804 | N | LEU | A | 536 | -0.203 | -9.645 | -14.299 | 1.00 | 53.63 |
| | ATOM | 1805 | CA | LEU | A | 536 | 0.382 | -10.926 | -13.937 | 1.00 | 53.11 |
| | ATOM | 1806 | CB | LEU | A | 536 | -0.250 | -12.046 | -14.763 | 1.00 | 51.88 |
| | ATOM | 1807 | CG | LEU | A | 536 | -0.686 | -13.256 | -13.938 | 1.00 | 51.83 |
| | ATOM | 1808 | CD1 | LEU | A | 536 | -1.953 | -12.917 | -13.173 | 1.00 | 49.51 |
| 60 | ATOM | 1809 | CD2 | LEU | A | 536 | -0.905 | -14.449 | -14.854 | 1.00 | 53.43 |
| | ATOM | 1810 | C | LEU | A | 536 | 1.895 | -10.990 | -14.081 | 1.00 | 52.58 |

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|----|------|------|-----|-----|---|-----|--------|---------|---------|------|-------|
| 5 | ATOM | 1811 | O | LEU | A | 536 | 2.414 | -11.501 | -15.075 | 1.00 | 55.33 |
| | ATOM | 1812 | N | TYR | A | 537 | 2.601 | -10.462 | -13.087 | 1.00 | 48.72 |
| | ATOM | 1813 | CA | TYR | A | 537 | 4.057 | -10.501 | -13.093 | 1.00 | 44.22 |
| | ATOM | 1814 | CB | TYR | A | 537 | 4.627 | -9.134 | -12.709 | 1.00 | 44.52 |
| | ATOM | 1815 | CG | TYR | A | 537 | 4.331 | -8.053 | -13.731 | 1.00 | 45.18 |
| 10 | ATOM | 1816 | CD1 | TYR | A | 537 | 3.623 | -6.905 | -13.376 | 1.00 | 43.77 |
| | ATOM | 1817 | CE1 | TYR | A | 537 | 3.334 | -5.915 | -14.317 | 1.00 | 45.23 |
| | ATOM | 1818 | CD2 | TYR | A | 537 | 4.747 | -8.187 | -15.058 | 1.00 | 46.91 |
| | ATOM | 1819 | CE2 | TYR | A | 537 | 4.462 | -7.202 | -16.008 | 1.00 | 43.93 |
| | ATOM | 1820 | CZ | TYR | A | 537 | 3.757 | -6.071 | -15.631 | 1.00 | 46.70 |
| 15 | ATOM | 1821 | OH | TYR | A | 537 | 3.472 | -5.097 | -16.565 | 1.00 | 48.35 |
| | ATOM | 1822 | C | TYR | A | 537 | 4.401 | -11.562 | -12.056 | 1.00 | 41.29 |
| | ATOM | 1823 | O | TYR | A | 537 | 4.330 | -11.319 | -10.856 | 1.00 | 41.82 |
| | ATOM | 1824 | N | ASP | A | 538 | 4.748 | -12.748 | -12.540 | 1.00 | 40.34 |
| | ATOM | 1825 | CA | ASP | A | 538 | 5.055 | -13.896 | -11.691 | 1.00 | 38.84 |
| 20 | ATOM | 1826 | CB | ASP | A | 538 | 5.594 | -15.037 | -12.554 | 1.00 | 43.47 |
| | ATOM | 1827 | CG | ASP | A | 538 | 4.571 | -15.531 | -13.566 | 1.00 | 47.67 |
| | ATOM | 1828 | OD1 | ASP | A | 538 | 4.931 | -16.373 | -14.416 | 1.00 | 49.33 |
| | ATOM | 1829 | OD2 | ASP | A | 538 | 3.405 | -15.073 | -13.511 | 1.00 | 48.07 |
| | ATOM | 1830 | C | ASP | A | 538 | 5.991 | -13.676 | -10.508 | 1.00 | 37.28 |
| 25 | ATOM | 1831 | O | ASP | A | 538 | 5.620 | -13.964 | -9.371 | 1.00 | 38.55 |
| | ATOM | 1832 | N | LEU | A | 539 | 7.196 | -13.200 | -10.766 | 1.00 | 33.83 |
| | ATOM | 1833 | CA | LEU | A | 539 | 8.155 | -12.959 | -9.692 | 1.00 | 32.80 |
| | ATOM | 1834 | CB | LEU | A | 539 | 9.419 | -12.323 | -10.263 | 1.00 | 32.78 |
| | ATOM | 1835 | CG | LEU | A | 539 | 10.561 | -12.031 | -9.292 | 1.00 | 30.93 |
| 30 | ATOM | 1836 | CD1 | LEU | A | 539 | 10.913 | -13.280 | -8.492 | 1.00 | 33.81 |
| | ATOM | 1837 | CD2 | LEU | A | 539 | 11.758 | -11.538 | -10.077 | 1.00 | 25.92 |
| | ATOM | 1838 | C | LEU | A | 539 | 7.558 | -12.050 | -8.614 | 1.00 | 31.85 |
| | ATOM | 1839 | O | LEU | A | 539 | 7.590 | -12.367 | -7.423 | 1.00 | 25.63 |
| | ATOM | 1840 | N | LEU | A | 540 | 7.011 | -10.917 | -9.042 | 1.00 | 32.07 |
| 35 | ATOM | 1841 | CA | LEU | A | 540 | 6.411 | -9.976 | -8.111 | 1.00 | 31.03 |
| | ATOM | 1842 | CB | LEU | A | 540 | 5.792 | -8.800 | -8.861 | 1.00 | 30.56 |
| | ATOM | 1843 | CG | LEU | A | 540 | 5.124 | -7.774 | -7.945 | 1.00 | 31.12 |
| | ATOM | 1844 | CD1 | LEU | A | 540 | 6.092 | -7.357 | -6.838 | 1.00 | 29.76 |
| | ATOM | 1845 | CD2 | LEU | A | 540 | 4.693 | -6.572 | -8.762 | 1.00 | 30.85 |
| 40 | ATOM | 1846 | C | LEU | A | 540 | 5.337 | -10.660 | -7.282 | 1.00 | 34.55 |
| | ATOM | 1847 | O | LEU | A | 540 | 5.316 | -10.522 | -6.063 | 1.00 | 31.60 |
| | ATOM | 1848 | N | LEU | A | 541 | 4.446 | -11.388 | -7.941 | 1.00 | 35.64 |
| | ATOM | 1849 | CA | LEU | A | 541 | 3.378 | -12.101 | -7.245 | 1.00 | 37.84 |
| | ATOM | 1850 | CB | LEU | A | 541 | 2.452 | -12.771 | -8.255 | 1.00 | 38.49 |
| 45 | ATOM | 1851 | CG | LEU | A | 541 | 1.244 | -11.932 | -8.678 | 1.00 | 39.80 |
| | ATOM | 1852 | CD1 | LEU | A | 541 | 0.476 | -11.476 | -7.448 | 1.00 | 40.02 |
| | ATOM | 1853 | CD2 | LEU | A | 541 | 1.713 | -10.733 | -9.485 | 1.00 | 40.48 |
| | ATOM | 1854 | C | LEU | A | 541 | 3.937 | -13.147 | -6.275 | 1.00 | 40.10 |
| | ATOM | 1855 | O | LEU | A | 541 | 3.472 | -13.254 | -5.137 | 1.00 | 42.72 |
| 50 | ATOM | 1856 | N | GLU | A | 542 | 4.929 | -13.915 | -6.723 | 1.00 | 38.45 |
| | ATOM | 1857 | CA | GLU | A | 542 | 5.535 | -14.932 | -5.868 | 1.00 | 39.59 |
| | ATOM | 1858 | CB | GLU | A | 542 | 6.738 | -15.566 | -6.564 | 1.00 | 41.73 |
| | ATOM | 1859 | CG | GLU | A | 542 | 6.396 | -16.327 | -7.831 | 1.00 | 48.34 |
| | ATOM | 1860 | CD | GLU | A | 542 | 6.931 | -17.747 | -7.819 | 1.00 | 52.57 |
| 55 | ATOM | 1861 | OE1 | GLU | A | 542 | 8.049 | -17.961 | -7.298 | 1.00 | 52.70 |
| | ATOM | 1862 | OE2 | GLU | A | 542 | 6.230 | -18.647 | -8.331 | 1.00 | 53.69 |
| | ATOM | 1863 | C | GLU | A | 542 | 5.989 | -14.299 | -4.553 | 1.00 | 39.94 |
| | ATOM | 1864 | O | GLU | A | 542 | 5.567 | -14.710 | -3.472 | 1.00 | 40.99 |
| | ATOM | 1865 | N | MET | A | 543 | 6.844 | -13.287 | -4.663 | 1.00 | 38.29 |
| 60 | ATOM | 1866 | CA | MET | A | 543 | 7.380 | -12.580 | -3.503 | 1.00 | 38.11 |
| | ATOM | 1867 | CB | MET | A | 543 | 8.242 | -11.408 | -3.963 | 1.00 | 37.34 |

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|----|--------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 1868 | CG | MET | A | 543 | 9.311 | -11.797 | -4.953 | 1.00 | 40.59 |
| | ATOM | 1869 | SD | MET | A | 543 | 10.829 | -12.223 | -4.114 | 1.00 | 45.64 |
| | ATOM | 1870 | CE | MET | A | 543 | 12.014 | -11.399 | -5.151 | 1.00 | 42.61 |
| | ATOM | 1871 | C | MET | A | 543 | 6.287 | -12.064 | -2.581 | 1.00 | 37.94 |
| | ATOM | 1872 | O | MET | A | 543 | 6.413 | -12.127 | -1.358 | 1.00 | 39.20 |
| 10 | ATOM | 1873 | N | LEU | A | 544 | 5.218 | -11.544 | -3.175 | 1.00 | 39.44 |
| | ATOM | 1874 | CA | LEU | A | 544 | 4.100 | -11.013 | -2.408 | 1.00 | 40.91 |
| | ATOM | 1875 | CB | LEU | A | 544 | 3.087 | -10.344 | -3.341 | 1.00 | 39.88 |
| | ATOM | 1876 | CG | LEU | A | 544 | 1.775 | -9.905 | -2.688 | 1.00 | 42.70 |
| | ATOM | 1877 | CD1 | LEU | A | 544 | 2.060 | -8.886 | -1.586 | 1.00 | 37.35 |
| 15 | ATOM | 1878 | CD2 | LEU | A | 544 | 0.854 | -9.317 | -3.741 | 1.00 | 38.47 |
| | ATOM | 1879 | C | LEU | A | 544 | 3.420 | -12.120 | -1.614 | 1.00 | 42.83 |
| | ATOM | 1880 | O | LEU | A | 544 | 2.957 | -11.899 | -0.496 | 1.00 | 42.73 |
| | ATOM | 1881 | N | ASP | A | 545 | 3.367 | -13.313 | -2.197 | 1.00 | 46.32 |
| | ATOM | 1882 | CA | ASP | A | 545 | 2.746 | -14.456 | -1.539 | 1.00 | 50.65 |
| 20 | ATOM | 1883 | CB | ASP | A | 545 | 2.606 | -15.617 | -2.524 | 1.00 | 53.67 |
| | ATOM | 1884 | CG | ASP | A | 545 | 1.703 | -15.278 | -3.691 | 1.00 | 57.35 |
| | ATOM | 1885 | OD1 | ASP | A | 545 | 0.697 | -14.568 | -3.475 | 1.00 | 59.99 |
| | ATOM | 1886 | OD2 | ASP | A | 545 | 1.999 | -15.718 | -4.824 | 1.00 | 59.68 |
| | ATOM | 1887 | C | ASP | A | 545 | 3.559 | -14.898 | -0.327 | 1.00 | 50.74 |
| 25 | ATOM | 1888 | O | ASP | A | 545 | 3.004 | -15.388 | 0.657 | 1.00 | 49.39 |
| | ATOM | 1889 | N | ALA | A | 546 | 4.874 | -14.723 | -0.401 | 1.00 | 51.82 |
| | ATOM | 1890 | CA | ALA | A | 546 | 5.750 | -15.095 | 0.702 | 1.00 | 53.12 |
| | ATOM | 1891 | CB | ALA | A | 546 | 7.180 | -14.678 | 0.395 | 1.00 | 53.19 |
| | ATOM | 1892 | C | ALA | A | 546 | 5.269 | -14.424 | 1.987 | 1.00 | 54.67 |
| 30 | ATOM | 1893 | O | ALA | A | 546 | 5.476 | -14.940 | 3.085 | 1.00 | 52.32 |
| | ATOM | 1894 | N | HIS | A | 547 | 4.622 | -13.270 | 1.838 | 1.00 | 56.66 |
| | ATOM | 1895 | CA | HIS | A | 547 | 4.102 | -12.520 | 2.978 | 1.00 | 59.19 |
| | ATOM | 1896 | CB | HIS | A | 547 | 4.144 | -11.017 | 2.684 | 1.00 | 56.70 |
| | ATOM | 1897 | CG | HIS | A | 547 | 5.489 | -10.394 | 2.896 | 1.00 | 54.64 |
| 35 | ATOM | 1898 | CD2 | HIS | A | 547 | 6.644 | -10.506 | 2.199 | 1.00 | 53.92 |
| | ATOM | 1899 | ND1 | HIS | A | 547 | 5.748 | -9.514 | 3.925 | 1.00 | 52.17 |
| | ATOM | 1900 | CE1 | HIS | A | 547 | 7.004 | -9.111 | 3.853 | 1.00 | 52.16 |
| | ATOM | 1901 | NE2 | HIS | A | 547 | 7.570 | -9.698 | 2.814 | 1.00 | 51.90 |
| | ATOM | 1902 | C | HIS | A | 547 | 2.668 | -12.940 | 3.306 | 1.00 | 62.77 |
| 40 | ATOM | 1903 | O | HIS | A | 547 | 1.842 | -12.120 | 3.707 | 1.00 | 63.24 |
| | ATOM | 1904 | N | ARG | A | 548 | 2.381 | -14.224 | 3.133 | 1.00 | 68.37 |
| | ATOM | 1905 | CA | ARG | A | 548 | 1.053 | -14.758 | 3.411 | 1.00 | 72.75 |
| | ATOM | 1906 | CB | ARG | A | 548 | 0.243 | -14.864 | 2.113 | 1.00 | 73.73 |
| | ATOM | 1907 | CG | ARG | A | 548 | -1.149 | -14.243 | 2.186 | 1.00 | 74.04 |
| 45 | ATOM | 1908 | CD | ARG | A | 548 | -1.081 | -12.728 | 2.297 | 1.00 | 74.50 |
| | ATOM | 1909 | NE | ARG | A | 548 | -2.305 | -12.167 | 2.863 | 1.00 | 75.04 |
| | ATOM | 1910 | CZ | ARG | A | 548 | -2.478 | -10.880 | 3.149 | 1.00 | 75.59 |
| | ATOM | 1911 | NH1 | ARG | A | 548 | -1.506 | -10.006 | 2.919 | 1.00 | 75.79 |
| | ATOM | 1912 | NH2 | ARG | A | 548 | -3.627 | -10.464 | 3.662 | 1.00 | 76.00 |
| 50 | ATOM | 1913 | C | ARG | A | 548 | 1.179 | -16.133 | 4.061 | 1.00 | 74.94 |
| | ATOM | 1914 | O | ARG | A | 548 | 0.197 | -16.697 | 4.549 | 1.00 | 75.15 |
| | ATOM | 1915 | N | LEU | A | 549 | 2.398 | -16.665 | 4.063 | 1.00 | 76.49 |
| | ATOM | 1916 | CA | LEU | A | 549 | 2.669 | -17.969 | 4.653 | 1.00 | 78.14 |
| | ATOM | 1917 | CB | LEU | A | 549 | 2.971 | -18.986 | 3.557 | 1.00 | 77.55 |
| 55 | ATOM | 1918 | C | LEU | A | 549 | 3.846 | -17.870 | 5.619 | 1.00 | 79.13 |
| | ATOM | 1919 | O | LEU | A | 549 | 4.892 | -17.317 | 5.215 | 1.00 | 80.40 |
| | ATOM | 1920 | OXT | LEU | A | 549 | 3.708 | -18.341 | 6.769 | 1.00 | 79.46 |
| | HETATM | 1921 | CP9 | DES | A | 600 | 5.390 | -3.061 | -6.139 | 1.00 | 21.38 |
| | HETATM | 1922 | CP8 | DES | A | 600 | 5.834 | -1.989 | -5.134 | 1.00 | 22.41 |
| 60 | HETATM | 1923 | CP7 | DES | A | 600 | 5.038 | -0.714 | -5.236 | 1.00 | 21.32 |
| | HETATM | 1924 | CP6 | DES | A | 600 | 3.587 | -0.864 | -5.062 | 1.00 | 25.87 |

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|----|--------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| 5 | HETATM | 1925 | CP1 | DES | A | 600 | 2.987 | -0.978 | -3.784 | 1.00 | 23.92 |
| | HETATM | 1926 | CP2 | DES | A | 600 | 1.597 | -1.150 | -3.684 | 1.00 | 29.77 |
| | HETATM | 1927 | CP3 | DES | A | 600 | 0.842 | -1.214 | -4.871 | 1.00 | 31.40 |
| | HETATM | 1928 | OP3 | DES | A | 600 | -0.506 | -1.419 | -4.824 | 1.00 | 33.36 |
| | HETATM | 1929 | CP4 | DES | A | 600 | 1.421 | -1.099 | -6.143 | 1.00 | 27.01 |
| 10 | HETATM | 1930 | CP5 | DES | A | 600 | 2.793 | -0.929 | -6.230 | 1.00 | 27.40 |
| | HETATM | 1931 | C7 | DES | A | 600 | 5.671 | 0.461 | -5.482 | 1.00 | 22.39 |
| | HETATM | 1932 | C6 | DES | A | 600 | 7.113 | 0.561 | -5.809 | 1.00 | 21.75 |
| | HETATM | 1933 | C5 | DES | A | 600 | 7.541 | 0.306 | -7.131 | 1.00 | 19.97 |
| | HETATM | 1934 | C4 | DES | A | 600 | 8.889 | 0.429 | -7.477 | 1.00 | 23.81 |
| 15 | HETATM | 1935 | C3 | DES | A | 600 | 9.814 | 0.804 | -6.488 | 1.00 | 21.88 |
| | HETATM | 1936 | O3 | DES | A | 600 | 11.125 | 0.901 | -6.839 | 1.00 | 22.32 |
| | HETATM | 1937 | C2 | DES | A | 600 | 9.423 | 1.066 | -5.161 | 1.00 | 19.74 |
| | HETATM | 1938 | C1 | DES | A | 600 | 8.066 | 0.937 | -4.838 | 1.00 | 21.25 |
| | HETATM | 1939 | C8 | DES | A | 600 | 4.894 | 1.765 | -5.443 | 1.00 | 21.47 |
| 20 | HETATM | 1940 | C9 | DES | A | 600 | 4.959 | 2.468 | -4.070 | 1.00 | 21.38 |
| | HETATM | 1941 | CL | CL | A | 601 | 14.781 | -3.035 | -17.739 | 1.00 | 24.10 |
| | ATOM | 1942 | CB | SER | B | 305 | 12.321 | 21.086 | 25.295 | 1.00 | 64.27 |
| | ATOM | 1943 | C | SER | B | 305 | 12.672 | 22.102 | 27.548 | 1.00 | 64.37 |
| | ATOM | 1944 | O | SER | B | 305 | 13.701 | 22.760 | 27.702 | 1.00 | 66.90 |
| 25 | ATOM | 1945 | N | SER | B | 305 | 12.045 | 23.521 | 25.606 | 1.00 | 63.72 |
| | ATOM | 1946 | CA | SER | B | 305 | 11.875 | 22.187 | 26.251 | 1.00 | 64.21 |
| | ATOM | 1947 | N | LEU | B | 306 | 12.193 | 21.293 | 28.484 | 1.00 | 63.09 |
| | ATOM | 1948 | CA | LEU | B | 306 | 12.884 | 21.133 | 29.757 | 1.00 | 60.98 |
| | ATOM | 1949 | CB | LEU | B | 306 | 11.884 | 21.200 | 30.913 | 1.00 | 61.23 |
| 30 | ATOM | 1950 | CG | LEU | B | 306 | 12.221 | 20.417 | 32.183 | 1.00 | 62.23 |
| | ATOM | 1951 | CD1 | LEU | B | 306 | 13.304 | 21.144 | 32.966 | 1.00 | 62.56 |
| | ATOM | 1952 | CD2 | LEU | B | 306 | 10.965 | 20.258 | 33.027 | 1.00 | 64.31 |
| | ATOM | 1953 | C | LEU | B | 306 | 13.660 | 19.819 | 29.803 | 1.00 | 58.39 |
| | ATOM | 1954 | O | LEU | B | 306 | 14.570 | 19.654 | 30.614 | 1.00 | 58.56 |
| 35 | ATOM | 1955 | N | ALA | B | 307 | 13.293 | 18.881 | 28.933 | 1.00 | 54.82 |
| | ATOM | 1956 | CA | ALA | B | 307 | 13.971 | 17.589 | 28.861 | 1.00 | 50.62 |
| | ATOM | 1957 | CB | ALA | B | 307 | 13.092 | 16.584 | 28.143 | 1.00 | 51.30 |
| | ATOM | 1958 | C | ALA | B | 307 | 15.303 | 17.719 | 28.122 | 1.00 | 46.84 |
| | ATOM | 1959 | O | ALA | B | 307 | 16.196 | 16.885 | 28.274 | 1.00 | 45.62 |
| 40 | ATOM | 1960 | N | LEU | B | 308 | 15.431 | 18.769 | 27.320 | 1.00 | 43.46 |
| | ATOM | 1961 | CA | LEU | B | 308 | 16.643 | 18.983 | 26.542 | 1.00 | 43.01 |
| | ATOM | 1962 | CB | LEU | B | 308 | 16.413 | 20.100 | 25.526 | 1.00 | 41.32 |
| | ATOM | 1963 | CG | LEU | B | 308 | 16.315 | 19.708 | 24.051 | 1.00 | 43.10 |
| | ATOM | 1964 | CD1 | LEU | B | 308 | 15.942 | 18.239 | 23.903 | 1.00 | 40.51 |
| 45 | ATOM | 1965 | CD2 | LEU | B | 308 | 15.287 | 20.602 | 23.375 | 1.00 | 39.80 |
| | ATOM | 1966 | C | LEU | B | 308 | 17.874 | 19.297 | 27.385 | 1.00 | 42.11 |
| | ATOM | 1967 | O | LEU | B | 308 | 19.000 | 19.102 | 26.932 | 1.00 | 44.34 |
| | ATOM | 1968 | N | SER | B | 309 | 17.669 | 19.775 | 28.608 | 1.00 | 40.88 |
| | ATOM | 1969 | CA | SER | B | 309 | 18.796 | 20.100 | 29.475 | 1.00 | 42.79 |
| 50 | ATOM | 1970 | CB | SER | B | 309 | 18.562 | 21.447 | 30.163 | 1.00 | 41.25 |
| | ATOM | 1971 | OG | SER | B | 309 | 17.459 | 21.379 | 31.046 | 1.00 | 46.67 |
| | ATOM | 1972 | C | SER | B | 309 | 19.072 | 19.028 | 30.529 | 1.00 | 42.60 |
| | ATOM | 1973 | O | SER | B | 309 | 20.053 | 19.119 | 31.269 | 1.00 | 44.18 |
| | ATOM | 1974 | N | LEU | B | 310 | 18.217 | 18.012 | 30.596 | 1.00 | 39.44 |
| 55 | ATOM | 1975 | CA | LEU | B | 310 | 18.394 | 16.936 | 31.569 | 1.00 | 37.62 |
| | ATOM | 1976 | CB | LEU | B | 310 | 17.205 | 15.969 | 31.499 | 1.00 | 38.84 |
| | ATOM | 1977 | CG | LEU | B | 310 | 16.216 | 15.873 | 32.668 | 1.00 | 42.43 |
| | ATOM | 1978 | CD1 | LEU | B | 310 | 16.040 | 17.219 | 33.355 | 1.00 | 42.55 |
| | ATOM | 1979 | CD2 | LEU | B | 310 | 14.881 | 15.380 | 32.138 | 1.00 | 39.69 |
| 60 | ATOM | 1980 | C | LEU | B | 310 | 19.691 | 16.174 | 31.285 | 1.00 | 34.11 |
| | ATOM | 1981 | O | LEU | B | 310 | 20.111 | 16.070 | 30.139 | 1.00 | 34.41 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1982 | N | THR | B | 311 | 20.339 | 15.662 | 32.326 | 1.00 | 34.04 |
| | ATOM | 1983 | CA | THR | B | 311 | 21.564 | 14.888 | 32.127 | 1.00 | 32.34 |
| | ATOM | 1984 | CB | THR | B | 311 | 22.434 | 14.824 | 33.399 | 1.00 | 31.75 |
| | ATOM | 1985 | OG1 | THR | B | 311 | 21.724 | 14.116 | 34.420 | 1.00 | 36.20 |
| | ATOM | 1986 | CG2 | THR | B | 311 | 22.782 | 16.212 | 33.893 | 1.00 | 31.05 |
| 10 | ATOM | 1987 | C | THR | B | 311 | 21.145 | 13.460 | 31.790 | 1.00 | 32.37 |
| | ATOM | 1988 | O | THR | B | 311 | 19.967 | 13.117 | 31.899 | 1.00 | 28.16 |
| | ATOM | 1989 | N | ALA | B | 312 | 22.106 | 12.628 | 31.396 | 1.00 | 33.23 |
| | ATOM | 1990 | CA | ALA | B | 312 | 21.811 | 11.237 | 31.053 | 1.00 | 35.63 |
| | ATOM | 1991 | CB | ALA | B | 312 | 23.077 | 10.527 | 30.577 | 1.00 | 34.00 |
| 15 | ATOM | 1992 | C | ALA | B | 312 | 21.210 | 10.489 | 32.240 | 1.00 | 34.29 |
| | ATOM | 1993 | O | ALA | B | 312 | 20.226 | 9.766 | 32.089 | 1.00 | 33.10 |
| | ATOM | 1994 | N | ASP | B | 313 | 21.800 | 10.665 | 33.419 | 1.00 | 33.90 |
| | ATOM | 1995 | CA | ASP | B | 313 | 21.304 | 9.994 | 34.615 | 1.00 | 34.19 |
| | ATOM | 1996 | CB | ASP | B | 313 | 22.258 | 10.219 | 35.788 | 1.00 | 42.09 |
| 20 | ATOM | 1997 | CG | ASP | B | 313 | 23.494 | 9.358 | 35.700 | 1.00 | 44.87 |
| | ATOM | 1998 | OD1 | ASP | B | 313 | 24.586 | 9.858 | 36.040 | 1.00 | 51.57 |
| | ATOM | 1999 | OD2 | ASP | B | 313 | 23.377 | 8.184 | 35.290 | 1.00 | 46.79 |
| | ATOM | 2000 | C | ASP | B | 313 | 19.925 | 10.520 | 34.971 | 1.00 | 31.99 |
| | ATOM | 2001 | O | ASP | B | 313 | 19.056 | 9.768 | 35.426 | 1.00 | 32.03 |
| 25 | ATOM | 2002 | N | GLN | B | 314 | 19.733 | 11.819 | 34.763 | 1.00 | 29.38 |
| | ATOM | 2003 | CA | GLN | B | 314 | 18.458 | 12.457 | 35.046 | 1.00 | 29.73 |
| | ATOM | 2004 | CB | GLN | B | 314 | 18.562 | 13.966 | 34.832 | 1.00 | 32.88 |
| | ATOM | 2005 | CG | GLN | B | 314 | 18.970 | 14.732 | 36.085 | 1.00 | 36.47 |
| | ATOM | 2006 | CD | GLN | B | 314 | 19.213 | 16.208 | 35.815 | 1.00 | 36.76 |
| 30 | ATOM | 2007 | OE1 | GLN | B | 314 | 19.300 | 16.634 | 34.664 | 1.00 | 38.79 |
| | ATOM | 2008 | NE2 | GLN | B | 314 | 19.327 | 16.995 | 36.880 | 1.00 | 39.72 |
| | ATOM | 2009 | C | GLN | B | 314 | 17.409 | 11.873 | 34.116 | 1.00 | 29.11 |
| | ATOM | 2010 | O | GLN | B | 314 | 16.274 | 11.620 | 34.522 | 1.00 | 28.82 |
| | ATOM | 2011 | N | MET | B | 315 | 17.801 | 11.657 | 32.864 | 1.00 | 27.27 |
| 35 | ATOM | 2012 | CA | MET | B | 315 | 16.900 | 11.079 | 31.872 | 1.00 | 30.41 |
| | ATOM | 2013 | CB | MET | B | 315 | 17.595 | 11.029 | 30.509 | 1.00 | 30.10 |
| | ATOM | 2014 | CG | MET | B | 315 | 16.787 | 10.345 | 29.421 | 1.00 | 38.02 |
| | ATOM | 2015 | SD | MET | B | 315 | 15.252 | 11.220 | 29.065 | 1.00 | 41.12 |
| | ATOM | 2016 | CE | MET | B | 315 | 15.890 | 12.835 | 28.611 | 1.00 | 39.32 |
| 40 | ATOM | 2017 | C | MET | B | 315 | 16.490 | 9.665 | 32.311 | 1.00 | 27.99 |
| | ATOM | 2018 | O | MET | B | 315 | 15.302 | 9.351 | 32.396 | 1.00 | 26.60 |
| | ATOM | 2019 | N | VAL | B | 316 | 17.481 | 8.823 | 32.598 | 1.00 | 27.26 |
| | ATOM | 2020 | CA | VAL | B | 316 | 17.229 | 7.447 | 33.027 | 1.00 | 24.54 |
| | ATOM | 2021 | CB | VAL | B | 316 | 18.554 | 6.708 | 33.351 | 1.00 | 26.22 |
| 45 | ATOM | 2022 | CG1 | VAL | B | 316 | 18.272 | 5.404 | 34.096 | 1.00 | 29.81 |
| | ATOM | 2023 | CG2 | VAL | B | 316 | 19.302 | 6.410 | 32.074 | 1.00 | 29.75 |
| | ATOM | 2024 | C | VAL | B | 316 | 16.326 | 7.389 | 34.258 | 1.00 | 27.22 |
| | ATOM | 2025 | O | VAL | B | 316 | 15.397 | 6.579 | 34.318 | 1.00 | 25.55 |
| | ATOM | 2026 | N | SER | B | 317 | 16.601 | 8.243 | 35.242 | 1.00 | 24.40 |
| 50 | ATOM | 2027 | CA | SER | B | 317 | 15.799 | 8.268 | 36.460 | 1.00 | 27.63 |
| | ATOM | 2028 | CB | SER | B | 317 | 16.358 | 9.294 | 37.451 | 1.00 | 31.68 |
| | ATOM | 2029 | OG | SER | B | 317 | 17.492 | 8.771 | 38.112 | 1.00 | 39.97 |
| | ATOM | 2030 | C | SER | B | 317 | 14.346 | 8.600 | 36.154 | 1.00 | 26.73 |
| | ATOM | 2031 | O | SER | B | 317 | 13.434 | 7.932 | 36.648 | 1.00 | 25.65 |
| 55 | ATOM | 2032 | N | ALA | B | 318 | 14.135 | 9.634 | 35.342 | 1.00 | 24.19 |
| | ATOM | 2033 | CA | ALA | B | 318 | 12.786 | 10.049 | 34.969 | 1.00 | 24.17 |
| | ATOM | 2034 | CB | ALA | B | 318 | 12.850 | 11.250 | 34.022 | 1.00 | 21.44 |
| | ATOM | 2035 | C | ALA | B | 318 | 12.038 | 8.890 | 34.306 | 1.00 | 21.63 |
| | ATOM | 2036 | O | ALA | B | 318 | 10.902 | 8.598 | 34.648 | 1.00 | 20.25 |
| 60 | ATOM | 2037 | N | LEU | B | 319 | 12.695 | 8.225 | 33.364 | 1.00 | 23.37 |
| | ATOM | 2038 | CA | LEU | B | 319 | 12.098 | 7.102 | 32.652 | 1.00 | 25.42 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 2039 | CB | LEU | B | 319 | 13.050 | 6.635 | 31.548 | 1.00 | 22.03 |
| | ATOM | 2040 | CG | LEU | B | 319 | 13.264 | 7.622 | 30.394 | 1.00 | 20.71 |
| | ATOM | 2041 | CD1 | LEU | B | 319 | 14.146 | 6.995 | 29.331 | 1.00 | 23.60 |
| | ATOM | 2042 | CD2 | LEU | B | 319 | 11.918 | 8.020 | 29.803 | 1.00 | 23.82 |
| | ATOM | 2043 | C | LEU | B | 319 | 11.729 | 5.926 | 33.564 | 1.00 | 27.26 |
| 10 | ATOM | 2044 | O | LEU | B | 319 | 10.615 | 5.396 | 33.488 | 1.00 | 28.91 |
| | ATOM | 2045 | N | LEU | B | 320 | 12.656 | 5.516 | 34.426 | 1.00 | 26.58 |
| | ATOM | 2046 | CA | LEU | B | 320 | 12.399 | 4.405 | 35.334 | 1.00 | 26.73 |
| | ATOM | 2047 | CB | LEU | B | 320 | 13.657 | 4.075 | 36.145 | 1.00 | 26.87 |
| | ATOM | 2048 | CG | LEU | B | 320 | 14.846 | 3.460 | 35.398 | 1.00 | 26.15 |
| 15 | ATOM | 2049 | CD1 | LEU | B | 320 | 16.053 | 3.375 | 36.330 | 1.00 | 28.04 |
| | ATOM | 2050 | CD2 | LEU | B | 320 | 14.484 | 2.076 | 34.895 | 1.00 | 26.96 |
| | ATOM | 2051 | C | LEU | B | 320 | 11.249 | 4.722 | 36.290 | 1.00 | 29.19 |
| | ATOM | 2052 | O | LEU | B | 320 | 10.449 | 3.849 | 36.631 | 1.00 | 26.66 |
| | ATOM | 2053 | N | ASP | B | 321 | 11.160 | 5.976 | 36.719 | 1.00 | 29.72 |
| 20 | ATOM | 2054 | CA | ASP | B | 321 | 10.112 | 6.371 | 37.647 | 1.00 | 31.36 |
| | ATOM | 2055 | CB | ASP | B | 321 | 10.494 | 7.683 | 38.336 | 1.00 | 36.60 |
| | ATOM | 2056 | CG | ASP | B | 321 | 11.407 | 7.461 | 39.535 | 1.00 | 46.11 |
| | ATOM | 2057 | OD1 | ASP | B | 321 | 10.897 | 7.058 | 40.605 | 1.00 | 46.64 |
| | ATOM | 2058 | OD2 | ASP | B | 321 | 12.635 | 7.676 | 39.402 | 1.00 | 45.98 |
| 25 | ATOM | 2059 | C | ASP | B | 321 | 8.742 | 6.494 | 36.989 | 1.00 | 28.29 |
| | ATOM | 2060 | O | ASP | B | 321 | 7.715 | 6.432 | 37.661 | 1.00 | 27.19 |
| | ATOM | 2061 | N | ALA | B | 322 | 8.726 | 6.650 | 35.672 | 1.00 | 28.34 |
| | ATOM | 2062 | CA | ALA | B | 322 | 7.469 | 6.779 | 34.950 | 1.00 | 25.55 |
| | ATOM | 2063 | CB | ALA | B | 322 | 7.668 | 7.668 | 33.728 | 1.00 | 24.11 |
| 30 | ATOM | 2064 | C | ALA | B | 322 | 6.911 | 5.420 | 34.523 | 1.00 | 22.80 |
| | ATOM | 2065 | O | ALA | B | 322 | 5.810 | 5.338 | 33.979 | 1.00 | 24.54 |
| | ATOM | 2066 | N | GLU | B | 323 | 7.662 | 4.355 | 34.781 | 1.00 | 20.16 |
| | ATOM | 2067 | CA | GLU | B | 323 | 7.229 | 3.021 | 34.386 | 1.00 | 21.44 |
| | ATOM | 2068 | CB | GLU | B | 323 | 8.196 | 1.982 | 34.938 | 1.00 | 23.72 |
| 35 | ATOM | 2069 | CG | GLU | B | 323 | 9.393 | 1.746 | 34.024 | 1.00 | 23.58 |
| | ATOM | 2070 | CD | GLU | B | 323 | 8.988 | 1.134 | 32.685 | 1.00 | 25.23 |
| | ATOM | 2071 | OE1 | GLU | B | 323 | 8.852 | 1.881 | 31.692 | 1.00 | 21.74 |
| | ATOM | 2072 | OE2 | GLU | B | 323 | 8.809 | -0.095 | 32.624 | 1.00 | 25.49 |
| | ATOM | 2073 | C | GLU | B | 323 | 5.796 | 2.696 | 34.810 | 1.00 | 22.35 |
| 40 | ATOM | 2074 | O | GLU | B | 323 | 5.409 | 2.926 | 35.951 | 1.00 | 22.34 |
| | ATOM | 2075 | N | PRO | B | 324 | 4.986 | 2.165 | 33.880 | 1.00 | 19.10 |
| | ATOM | 2076 | CD | PRO | B | 324 | 5.286 | 1.806 | 32.483 | 1.00 | 19.11 |
| | ATOM | 2077 | CA | PRO | B | 324 | 3.607 | 1.839 | 34.242 | 1.00 | 22.04 |
| | ATOM | 2078 | CB | PRO | B | 324 | 2.919 | 1.658 | 32.893 | 1.00 | 21.96 |
| 45 | ATOM | 2079 | CG | PRO | B | 324 | 4.015 | 1.137 | 32.015 | 1.00 | 24.13 |
| | ATOM | 2080 | C | PRO | B | 324 | 3.619 | 0.556 | 35.060 | 1.00 | 23.44 |
| | ATOM | 2081 | O | PRO | B | 324 | 4.590 | -0.200 | 35.028 | 1.00 | 22.20 |
| | ATOM | 2082 | N | PRO | B | 325 | 2.540 | 0.287 | 35.801 | 1.00 | 24.88 |
| | ATOM | 2083 | CD | PRO | B | 325 | 1.299 | 1.068 | 35.945 | 1.00 | 26.67 |
| 50 | ATOM | 2084 | CA | PRO | B | 325 | 2.520 | -0.940 | 36.603 | 1.00 | 25.10 |
| | ATOM | 2085 | CB | PRO | B | 325 | 1.394 | -0.691 | 37.595 | 1.00 | 27.09 |
| | ATOM | 2086 | CG | PRO | B | 325 | 0.448 | 0.205 | 36.854 | 1.00 | 26.87 |
| | ATOM | 2087 | C | PRO | B | 325 | 2.270 | -2.192 | 35.776 | 1.00 | 25.77 |
| | ATOM | 2088 | O | PRO | B | 325 | 1.853 | -2.118 | 34.617 | 1.00 | 21.69 |
| 55 | ATOM | 2089 | N | ILE | B | 326 | 2.538 | -3.344 | 36.379 | 1.00 | 24.05 |
| | ATOM | 2090 | CA | ILE | B | 326 | 2.301 | -4.620 | 35.722 | 1.00 | 22.51 |
| | ATOM | 2091 | CB | ILE | B | 326 | 3.303 | -5.688 | 36.185 | 1.00 | 25.81 |
| | ATOM | 2092 | CG2 | ILE | B | 326 | 3.011 | -7.018 | 35.481 | 1.00 | 23.78 |
| | ATOM | 2093 | CG1 | ILE | B | 326 | 4.729 | -5.209 | 35.900 | 1.00 | 25.75 |
| 60 | ATOM | 2094 | CD1 | ILE | B | 326 | 5.241 | -5.585 | 34.533 | 1.00 | 27.78 |
| | ATOM | 2095 | C | ILE | B | 326 | 0.893 | -5.020 | 36.149 | 1.00 | 23.63 |

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|----|------|------|-----|-----|---|-----|---------|---------|--------|------|-------|
| 5 | ATOM | 2096 | O | ILE | B | 326 | 0.632 | -5.231 | 37.332 | 1.00 | 24.81 |
| | ATOM | 2097 | N | LEU | B | 327 | -0.018 | -5.104 | 35.188 | 1.00 | 19.44 |
| | ATOM | 2098 | CA | LEU | B | 327 | -1.399 | -5.437 | 35.493 | 1.00 | 17.03 |
| | ATOM | 2099 | CB | LEU | B | 327 | -2.336 | -4.747 | 34.493 | 1.00 | 18.39 |
| | ATOM | 2100 | CG | LEU | B | 327 | -2.201 | -3.216 | 34.373 | 1.00 | 20.69 |
| 10 | ATOM | 2101 | CD1 | LEU | B | 327 | -3.245 | -2.679 | 33.406 | 1.00 | 14.87 |
| | ATOM | 2102 | CD2 | LEU | B | 327 | -2.384 | -2.570 | 35.742 | 1.00 | 14.39 |
| | ATOM | 2103 | C | LEU | B | 327 | -1.662 | -6.928 | 35.499 | 1.00 | 19.87 |
| | ATOM | 2104 | O | LEU | B | 327 | -0.854 | -7.722 | 35.014 | 1.00 | 20.90 |
| | ATOM | 2105 | N | TYR | B | 328 | -2.803 | -7.300 | 36.066 | 1.00 | 20.92 |
| 15 | ATOM | 2106 | CA | TYR | B | 328 | -3.202 | -8.692 | 36.135 | 1.00 | 21.79 |
| | ATOM | 2107 | CB | TYR | B | 328 | -3.658 | -9.050 | 37.550 | 1.00 | 22.91 |
| | ATOM | 2108 | CG | TYR | B | 328 | -2.515 | -9.376 | 38.468 | 1.00 | 24.60 |
| | ATOM | 2109 | CD1 | TYR | B | 328 | -2.118 | -10.696 | 38.677 | 1.00 | 25.93 |
| | ATOM | 2110 | CE1 | TYR | B | 328 | -1.034 | -11.000 | 39.498 | 1.00 | 28.10 |
| 20 | ATOM | 2111 | CD2 | TYR | B | 328 | -1.802 | -8.362 | 39.103 | 1.00 | 29.46 |
| | ATOM | 2112 | CE2 | TYR | B | 328 | -0.716 | -8.654 | 39.926 | 1.00 | 35.30 |
| | ATOM | 2113 | CZ | TYR | B | 328 | -0.338 | -9.973 | 40.117 | 1.00 | 32.59 |
| | ATOM | 2114 | OH | TYR | B | 328 | 0.739 | -10.257 | 40.923 | 1.00 | 37.24 |
| | ATOM | 2115 | C | TYR | B | 328 | -4.336 | -8.944 | 35.168 | 1.00 | 22.25 |
| 25 | ATOM | 2116 | O | TYR | B | 328 | -5.115 | -8.039 | 34.849 | 1.00 | 19.77 |
| | ATOM | 2117 | N | SER | B | 329 | -4.420 | -10.180 | 34.698 | 1.00 | 25.81 |
| | ATOM | 2118 | CA | SER | B | 329 | -5.480 | -10.571 | 33.787 | 1.00 | 29.39 |
| | ATOM | 2119 | CB | SER | B | 329 | -5.002 | -11.710 | 32.887 | 1.00 | 27.65 |
| | ATOM | 2120 | OG | SER | B | 329 | -6.091 | -12.329 | 32.233 | 1.00 | 28.98 |
| 30 | ATOM | 2121 | C | SER | B | 329 | -6.625 | -11.042 | 34.673 | 1.00 | 33.17 |
| | ATOM | 2122 | O | SER | B | 329 | -6.453 | -11.157 | 35.888 | 1.00 | 32.52 |
| | ATOM | 2123 | N | GLU | B | 330 | -7.792 | -11.289 | 34.084 | 1.00 | 38.75 |
| | ATOM | 2124 | CA | GLU | B | 330 | -8.930 | -11.776 | 34.859 | 1.00 | 44.91 |
| | ATOM | 2125 | CB | GLU | B | 330 | -10.134 | -11.999 | 33.951 | 1.00 | 45.63 |
| 35 | ATOM | 2126 | C | GLU | B | 330 | -8.493 | -13.093 | 35.491 | 1.00 | 48.62 |
| | ATOM | 2127 | O | GLU | B | 330 | -7.739 | -13.851 | 34.882 | 1.00 | 52.37 |
| | ATOM | 2128 | N | TYR | B | 331 | -8.952 | -13.366 | 36.707 | 1.00 | 51.75 |
| | ATOM | 2129 | CA | TYR | B | 331 | -8.575 | -14.596 | 37.396 | 1.00 | 55.25 |
| | ATOM | 2130 | CB | TYR | B | 331 | -8.538 | -14.365 | 38.911 | 1.00 | 53.04 |
| 40 | ATOM | 2131 | CG | TYR | B | 331 | -9.769 | -13.668 | 39.440 | 1.00 | 50.70 |
| | ATOM | 2132 | CD1 | TYR | B | 331 | -10.880 | -14.400 | 39.856 | 1.00 | 47.09 |
| | ATOM | 2133 | CE1 | TYR | B | 331 | -12.035 | -13.762 | 40.292 | 1.00 | 46.43 |
| | ATOM | 2134 | CD2 | TYR | B | 331 | -9.842 | -12.273 | 39.478 | 1.00 | 47.52 |
| | ATOM | 2135 | CE2 | TYR | B | 331 | -10.993 | -11.625 | 39.913 | 1.00 | 43.98 |
| 45 | ATOM | 2136 | CZ | TYR | B | 331 | -12.086 | -12.376 | 40.314 | 1.00 | 44.33 |
| | ATOM | 2137 | OH | TYR | B | 331 | -13.239 | -11.747 | 40.715 | 1.00 | 45.31 |
| | ATOM | 2138 | C | TYR | B | 331 | -9.528 | -15.743 | 37.075 | 1.00 | 60.11 |
| | ATOM | 2139 | O | TYR | B | 331 | -10.748 | -15.569 | 37.066 | 1.00 | 63.13 |
| 50 | ATOM | 2140 | N | ASP | B | 332 | -8.952 | -16.913 | 36.809 | 1.00 | 61.60 |
| | ATOM | 2141 | CA | ASP | B | 332 | -9.704 | -18.124 | 36.490 | 1.00 | 63.58 |
| | ATOM | 2142 | CB | ASP | B | 332 | -10.637 | -17.895 | 35.298 | 1.00 | 65.11 |
| | ATOM | 2143 | CG | ASP | B | 332 | -11.723 | -18.953 | 35.200 | 1.00 | 65.32 |
| | ATOM | 2144 | OD1 | ASP | B | 332 | -11.420 | -20.136 | 35.463 | 1.00 | 63.69 |
| | ATOM | 2145 | OD2 | ASP | B | 332 | -12.876 | -18.602 | 34.866 | 1.00 | 63.61 |
| 55 | ATOM | 2146 | C | ASP | B | 332 | -8.707 | -19.227 | 36.153 | 1.00 | 62.86 |
| | ATOM | 2147 | O | ASP | B | 332 | -7.853 | -19.056 | 35.287 | 1.00 | 62.26 |
| | ATOM | 2148 | N | PRO | B | 333 | -8.811 | -20.379 | 36.833 | 1.00 | 63.96 |
| | ATOM | 2149 | CD | PRO | B | 333 | -9.808 | -20.690 | 37.875 | 1.00 | 64.24 |
| | ATOM | 2150 | CA | PRO | B | 333 | -7.901 | -21.503 | 36.596 | 1.00 | 64.24 |
| 60 | ATOM | 2151 | CB | PRO | B | 333 | -8.015 | -22.325 | 37.874 | 1.00 | 64.70 |
| | ATOM | 2152 | CG | PRO | B | 333 | -9.410 | -22.071 | 38.347 | 1.00 | 65.00 |

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|----|------|------|-----|-----|---|-----|---------|---------|--------|------|-------|
| 5 | ATOM | 2153 | C | PRO | B | 333 | -8.180 | -22.340 | 35.351 | 1.00 | 63.90 |
| | ATOM | 2154 | O | PRO | B | 333 | -7.384 | -23.214 | 35.007 | 1.00 | 63.70 |
| | ATOM | 2155 | N | THR | B | 334 | -9.303 | -22.084 | 34.683 | 1.00 | 63.83 |
| | ATOM | 2156 | CA | THR | B | 334 | -9.649 | -22.832 | 33.475 | 1.00 | 63.77 |
| | ATOM | 2157 | CB | THR | B | 334 | -11.065 | -22.477 | 32.975 | 1.00 | 64.63 |
| 10 | ATOM | 2158 | OG1 | THR | B | 334 | -11.132 | -21.078 | 32.675 | 1.00 | 65.95 |
| | ATOM | 2159 | CG2 | THR | B | 334 | -12.102 | -22.817 | 34.036 | 1.00 | 65.09 |
| | ATOM | 2160 | C | THR | B | 334 | -8.634 | -22.499 | 32.388 | 1.00 | 62.62 |
| | ATOM | 2161 | O | THR | B | 334 | -8.931 | -21.774 | 31.437 | 1.00 | 60.15 |
| | ATOM | 2162 | N | ARG | B | 335 | -7.432 | -23.043 | 32.553 | 1.00 | 63.14 |
| 15 | ATOM | 2163 | CA | ARG | B | 335 | -6.324 | -22.820 | 31.633 | 1.00 | 60.70 |
| | ATOM | 2164 | CB | ARG | B | 335 | -5.130 | -23.667 | 32.050 | 1.00 | 58.73 |
| | ATOM | 2165 | C | ARG | B | 335 | -6.667 | -23.086 | 30.174 | 1.00 | 59.71 |
| | ATOM | 2166 | O | ARG | B | 335 | -6.302 | -22.298 | 29.298 | 1.00 | 62.33 |
| | ATOM | 2167 | N | PRO | B | 336 | -7.377 | -24.194 | 29.884 | 1.00 | 55.25 |
| 20 | ATOM | 2168 | CD | PRO | B | 336 | -7.938 | -25.227 | 30.769 | 1.00 | 53.53 |
| | ATOM | 2169 | CA | PRO | B | 336 | -7.698 | -24.437 | 28.471 | 1.00 | 50.10 |
| | ATOM | 2170 | CB | PRO | B | 336 | -8.399 | -25.799 | 28.476 | 1.00 | 49.70 |
| | ATOM | 2171 | CG | PRO | B | 336 | -8.164 | -26.372 | 29.844 | 1.00 | 50.71 |
| | ATOM | 2172 | C | PRO | B | 336 | -8.602 | -23.324 | 27.954 | 1.00 | 44.54 |
| 25 | ATOM | 2173 | O | PRO | B | 336 | -9.809 | -23.342 | 28.179 | 1.00 | 44.14 |
| | ATOM | 2174 | N | PHE | B | 337 | -8.007 | -22.350 | 27.274 | 1.00 | 39.18 |
| | ATOM | 2175 | CA | PHE | B | 337 | -8.764 | -21.223 | 26.742 | 1.00 | 38.25 |
| | ATOM | 2176 | CB | PHE | B | 337 | -7.850 | -20.003 | 26.567 | 1.00 | 36.98 |
| | ATOM | 2177 | CG | PHE | B | 337 | -7.229 | -19.517 | 27.846 | 1.00 | 36.81 |
| 30 | ATOM | 2178 | CD1 | PHE | B | 337 | -5.846 | -19.511 | 28.002 | 1.00 | 38.89 |
| | ATOM | 2179 | CD2 | PHE | B | 337 | -8.023 | -19.062 | 28.893 | 1.00 | 35.97 |
| | ATOM | 2180 | CE1 | PHE | B | 337 | -5.262 | -19.059 | 29.185 | 1.00 | 36.85 |
| | ATOM | 2181 | CE2 | PHE | B | 337 | -7.449 | -18.608 | 30.079 | 1.00 | 37.15 |
| | ATOM | 2182 | CZ | PHE | B | 337 | -6.064 | -18.607 | 30.224 | 1.00 | 38.40 |
| 35 | ATOM | 2183 | C | PHE | B | 337 | -9.420 | -21.535 | 25.402 | 1.00 | 36.81 |
| | ATOM | 2184 | O | PHE | B | 337 | -8.962 | -22.399 | 24.658 | 1.00 | 36.26 |
| | ATOM | 2185 | N | SER | B | 338 | -10.504 | -20.828 | 25.107 | 1.00 | 35.85 |
| | ATOM | 2186 | CA | SER | B | 338 | -11.198 | -20.981 | 23.836 | 1.00 | 34.76 |
| | ATOM | 2187 | CB | SER | B | 338 | -12.713 | -20.948 | 24.035 | 1.00 | 34.85 |
| 40 | ATOM | 2188 | OG | SER | B | 338 | -13.164 | -19.621 | 24.235 | 1.00 | 33.53 |
| | ATOM | 2189 | C | SER | B | 338 | -10.761 | -19.761 | 23.037 | 1.00 | 34.99 |
| | ATOM | 2190 | O | SER | B | 338 | -10.143 | -18.855 | 23.591 | 1.00 | 34.32 |
| | ATOM | 2191 | N | GLU | B | 339 | -11.075 | -19.722 | 21.750 | 1.00 | 33.01 |
| | ATOM | 2192 | CA | GLU | B | 339 | -10.682 | -18.579 | 20.950 | 1.00 | 33.94 |
| 45 | ATOM | 2193 | CB | GLU | B | 339 | -11.146 | -18.737 | 19.501 | 1.00 | 33.79 |
| | ATOM | 2194 | CG | GLU | B | 339 | -10.758 | -17.553 | 18.623 | 1.00 | 39.11 |
| | ATOM | 2195 | CD | GLU | B | 339 | -10.865 | -17.852 | 17.137 | 1.00 | 43.17 |
| | ATOM | 2196 | OE1 | GLU | B | 339 | -11.990 | -17.785 | 16.600 | 1.00 | 45.28 |
| | ATOM | 2197 | OE2 | GLU | B | 339 | -9.824 | -18.152 | 16.510 | 1.00 | 39.19 |
| 50 | ATOM | 2198 | C | GLU | B | 339 | -11.265 | -17.295 | 21.531 | 1.00 | 34.28 |
| | ATOM | 2199 | O | GLU | B | 339 | -10.575 | -16.283 | 21.631 | 1.00 | 33.65 |
| | ATOM | 2200 | N | ALA | B | 340 | -12.535 | -17.339 | 21.920 | 1.00 | 31.12 |
| | ATOM | 2201 | CA | ALA | B | 340 | -13.194 | -16.164 | 22.469 | 1.00 | 29.10 |
| | ATOM | 2202 | CB | ALA | B | 340 | -14.696 | -16.412 | 22.573 | 1.00 | 33.84 |
| 55 | ATOM | 2203 | C | ALA | B | 340 | -12.639 | -15.731 | 23.826 | 1.00 | 28.98 |
| | ATOM | 2204 | O | ALA | B | 340 | -12.431 | -14.541 | 24.060 | 1.00 | 30.48 |
| | ATOM | 2205 | N | SER | B | 341 | -12.407 | -16.691 | 24.719 | 1.00 | 26.66 |
| | ATOM | 2206 | CA | SER | B | 341 | -11.882 | -16.386 | 26.044 | 1.00 | 24.26 |
| | ATOM | 2207 | CB | SER | B | 341 | -11.867 | -17.643 | 26.923 | 1.00 | 27.04 |
| 60 | ATOM | 2208 | OG | SER | B | 341 | -10.851 | -18.541 | 26.515 | 1.00 | 33.84 |
| | ATOM | 2209 | C | SER | B | 341 | -10.479 | -15.793 | 25.960 | 1.00 | 23.97 |

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|----|------|------|-----|-----|---|-----|---------|---------|--------|------|-------|
| 5 | ATOM | 2210 | O | SER | B | 341 | -10.171 | -14.824 | 26.651 | 1.00 | 21.56 |
| | ATOM | 2211 | N | MET | B | 342 | -9.631 | -16.368 | 25.114 | 1.00 | 26.83 |
| | ATOM | 2212 | CA | MET | B | 342 | -8.271 | -15.865 | 24.954 | 1.00 | 27.24 |
| | ATOM | 2213 | CB | MET | B | 342 | -7.477 | -16.758 | 24.001 | 1.00 | 30.45 |
| | ATOM | 2214 | CG | MET | B | 342 | -6.038 | -16.300 | 23.802 | 1.00 | 35.35 |
| 10 | ATOM | 2215 | SD | MET | B | 342 | -4.866 | -17.667 | 23.777 | 1.00 | 44.57 |
| | ATOM | 2216 | CE | MET | B | 342 | -4.034 | -17.341 | 22.244 | 1.00 | 41.37 |
| | ATOM | 2217 | C | MET | B | 342 | -8.322 | -14.448 | 24.385 | 1.00 | 25.31 |
| | ATOM | 2218 | O | MET | B | 342 | -7.653 | -13.541 | 24.874 | 1.00 | 26.67 |
| | ATOM | 2219 | N | MET | B | 343 | -9.114 | -14.278 | 23.345 | 1.00 | 25.75 |
| 15 | ATOM | 2220 | CA | MET | B | 343 | -9.262 | -12.979 | 22.712 | 1.00 | 25.47 |
| | ATOM | 2221 | CB | MET | B | 343 | -10.210 | -13.088 | 21.528 | 1.00 | 23.51 |
| | ATOM | 2222 | CG | MET | B | 343 | -9.540 | -13.618 | 20.273 | 1.00 | 28.86 |
| | ATOM | 2223 | SD | MET | B | 343 | -8.325 | -12.456 | 19.609 | 1.00 | 29.25 |
| | ATOM | 2224 | CE | MET | B | 343 | -9.344 | -11.015 | 19.371 | 1.00 | 28.74 |
| 20 | ATOM | 2225 | C | MET | B | 343 | -9.798 | -11.966 | 23.712 | 1.00 | 25.37 |
| | ATOM | 2226 | O | MET | B | 343 | -9.360 | -10.810 | 23.728 | 1.00 | 24.98 |
| | ATOM | 2227 | N | GLY | B | 344 | -10.739 | -12.403 | 24.536 | 1.00 | 23.91 |
| | ATOM | 2228 | CA | GLY | B | 344 | -11.320 | -11.526 | 25.536 | 1.00 | 22.43 |
| | ATOM | 2229 | C | GLY | B | 344 | -10.313 | -11.103 | 26.592 | 1.00 | 22.06 |
| 25 | ATOM | 2230 | O | GLY | B | 344 | -10.262 | -9.934 | 26.982 | 1.00 | 20.87 |
| | ATOM | 2231 | N | LEU | B | 345 | -9.511 | -12.048 | 27.063 | 1.00 | 19.36 |
| | ATOM | 2232 | CA | LEU | B | 345 | -8.520 | -11.748 | 28.083 | 1.00 | 25.74 |
| | ATOM | 2233 | CB | LEU | B | 345 | -7.886 | -13.040 | 28.600 | 1.00 | 26.78 |
| | ATOM | 2234 | CG | LEU | B | 345 | -8.794 | -14.010 | 29.362 | 1.00 | 30.04 |
| 30 | ATOM | 2235 | CD1 | LEU | B | 345 | -8.099 | -15.357 | 29.488 | 1.00 | 28.39 |
| | ATOM | 2236 | CD2 | LEU | B | 345 | -9.122 | -13.443 | 30.736 | 1.00 | 29.93 |
| | ATOM | 2237 | C | LEU | B | 345 | -7.425 | -10.822 | 27.550 | 1.00 | 23.24 |
| | ATOM | 2238 | O | LEU | B | 345 | -7.037 | -9.865 | 28.212 | 1.00 | 23.43 |
| | ATOM | 2239 | N | LEU | B | 346 | -6.937 | -11.108 | 26.350 | 1.00 | 21.92 |
| 35 | ATOM | 2240 | CA | LEU | B | 346 | -5.874 | -10.303 | 25.763 | 1.00 | 22.71 |
| | ATOM | 2241 | CB | LEU | B | 346 | -5.343 | -10.962 | 24.486 | 1.00 | 23.17 |
| | ATOM | 2242 | CG | LEU | B | 346 | -4.684 | -12.331 | 24.668 | 1.00 | 20.66 |
| | ATOM | 2243 | CD1 | LEU | B | 346 | -4.303 | -12.916 | 23.309 | 1.00 | 18.75 |
| | ATOM | 2244 | CD2 | LEU | B | 346 | -3.464 | -12.188 | 25.553 | 1.00 | 20.84 |
| 40 | ATOM | 2245 | C | LEU | B | 346 | -6.304 | -8.873 | 25.458 | 1.00 | 22.99 |
| | ATOM | 2246 | O | LEU | B | 346 | -5.540 | -7.935 | 25.695 | 1.00 | 22.07 |
| | ATOM | 2247 | N | THR | B | 347 | -7.516 | -8.699 | 24.937 | 1.00 | 20.53 |
| | ATOM | 2248 | CA | THR | B | 347 | -7.987 | -7.357 | 24.608 | 1.00 | 21.89 |
| | ATOM | 2249 | CB | THR | B | 347 | -9.152 | -7.388 | 23.601 | 1.00 | 21.65 |
| 45 | ATOM | 2250 | OG1 | THR | B | 347 | -10.218 | -8.190 | 24.123 | 1.00 | 19.65 |
| | ATOM | 2251 | CG2 | THR | B | 347 | -8.676 | -7.955 | 22.262 | 1.00 | 22.01 |
| | ATOM | 2252 | C | THR | B | 347 | -8.426 | -6.590 | 25.853 | 1.00 | 23.60 |
| | ATOM | 2253 | O | THR | B | 347 | -8.358 | -5.357 | 25.883 | 1.00 | 20.31 |
| | ATOM | 2254 | N | ASN | B | 348 | -8.884 | -7.314 | 26.874 | 1.00 | 22.27 |
| 50 | ATOM | 2255 | CA | ASN | B | 348 | -9.293 | -6.667 | 28.114 | 1.00 | 23.99 |
| | ATOM | 2256 | CB | ASN | B | 348 | -10.008 | -7.642 | 29.056 | 1.00 | 22.32 |
| | ATOM | 2257 | CG | ASN | B | 348 | -10.342 | -7.022 | 30.398 | 1.00 | 28.26 |
| | ATOM | 2258 | OD1 | ASN | B | 348 | -9.478 | -6.746 | 31.216 | 1.00 | 27.14 |
| | ATOM | 2259 | ND2 | ASN | B | 348 | -11.647 | -6.764 | 30.625 | 1.00 | 27.02 |
| 55 | ATOM | 2260 | C | ASN | B | 348 | -8.035 | -6.120 | 28.798 | 1.00 | 19.48 |
| | ATOM | 2261 | O | ASN | B | 348 | -8.014 | -4.991 | 29.271 | 1.00 | 18.26 |
| | ATOM | 2262 | N | LEU | B | 349 | -6.984 | -6.931 | 28.832 | 1.00 | 19.07 |
| | ATOM | 2263 | CA | LEU | B | 349 | -5.724 | -6.516 | 29.446 | 1.00 | 20.37 |
| | ATOM | 2264 | CB | LEU | B | 349 | -4.716 | -7.674 | 29.434 | 1.00 | 18.21 |
| 60 | ATOM | 2265 | CG | LEU | B | 349 | -3.297 | -7.316 | 29.889 | 1.00 | 18.24 |
| | ATOM | 2266 | CD1 | LEU | B | 349 | -3.323 | -6.904 | 31.356 | 1.00 | 12.44 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|
| 5 | ATOM | 2267 | CD2 | LEU | B | 349 | -2.370 | -8.504 | 29.672 | 1.00 | 21.28 |
| | ATOM | 2268 | C | LEU | B | 349 | -5.131 | -5.307 | 28.718 | 1.00 | 19.92 |
| | ATOM | 2269 | O | LEU | B | 349 | -4.738 | -4.322 | 29.349 | 1.00 | 16.56 |
| | ATOM | 2270 | N | ALA | B | 350 | -5.067 | -5.391 | 27.391 | 1.00 | 16.67 |
| | ATOM | 2271 | CA | ALA | B | 350 | -4.529 | -4.308 | 26.578 | 1.00 | 17.11 |
| 10 | ATOM | 2272 | CB | ALA | B | 350 | -4.587 | -4.690 | 25.095 | 1.00 | 14.15 |
| | ATOM | 2273 | C | ALA | B | 350 | -5.272 | -2.988 | 26.805 | 1.00 | 17.92 |
| | ATOM | 2274 | O | ALA | B | 350 | -4.650 | -1.926 | 26.904 | 1.00 | 18.71 |
| | ATOM | 2275 | N | ASP | B | 351 | -6.600 | -3.053 | 26.857 | 1.00 | 17.51 |
| | ATOM | 2276 | CA | ASP | B | 351 | -7.409 | -1.856 | 27.074 | 1.00 | 16.57 |
| 15 | ATOM | 2277 | CB | ASP | B | 351 | -8.902 | -2.202 | 27.041 | 1.00 | 18.97 |
| | ATOM | 2278 | CG | ASP | B | 351 | -9.785 | -0.974 | 26.858 | 1.00 | 21.80 |
| | ATOM | 2279 | OD1 | ASP | B | 351 | -9.660 | -0.292 | 25.824 | 1.00 | 24.62 |
| | ATOM | 2280 | OD2 | ASP | B | 351 | -10.604 | -0.682 | 27.754 | 1.00 | 22.78 |
| | ATOM | 2281 | C | ASP | B | 351 | -7.064 | -1.228 | 28.415 | 1.00 | 16.81 |
| 20 | ATOM | 2282 | O | ASP | B | 351 | -6.963 | -0.009 | 28.534 | 1.00 | 15.75 |
| | ATOM | 2283 | N | ARG | B | 352 | -6.894 | -2.056 | 29.438 | 1.00 | 13.97 |
| | ATOM | 2284 | CA | ARG | B | 352 | -6.552 | -1.509 | 30.742 | 1.00 | 16.09 |
| | ATOM | 2285 | CB | ARG | B | 352 | -6.728 | -2.571 | 31.833 | 1.00 | 15.78 |
| | ATOM | 2286 | CG | ARG | B | 352 | -8.189 | -2.819 | 32.189 | 1.00 | 17.93 |
| 25 | ATOM | 2287 | CD | ARG | B | 352 | -8.323 | -3.882 | 33.279 | 1.00 | 19.84 |
| | ATOM | 2288 | NE | ARG | B | 352 | -8.010 | -5.222 | 32.785 | 1.00 | 21.36 |
| | ATOM | 2289 | CZ | ARG | B | 352 | -7.187 | -6.075 | 33.387 | 1.00 | 21.18 |
| | ATOM | 2290 | NH1 | ARG | B | 352 | -6.579 | -5.741 | 34.516 | 1.00 | 20.51 |
| | ATOM | 2291 | NH2 | ARG | B | 352 | -6.980 | -7.275 | 32.864 | 1.00 | 28.51 |
| 30 | ATOM | 2292 | C | ARG | B | 352 | -5.123 | -0.975 | 30.728 | 1.00 | 15.81 |
| | ATOM | 2293 | O | ARG | B | 352 | -4.835 | 0.057 | 31.339 | 1.00 | 15.61 |
| | ATOM | 2294 | N | GLU | B | 353 | -4.231 | -1.665 | 30.019 | 1.00 | 15.45 |
| | ATOM | 2295 | CA | GLU | B | 353 | -2.838 | -1.228 | 29.935 | 1.00 | 16.59 |
| | ATOM | 2296 | CB | GLU | B | 353 | -1.990 | -2.243 | 29.168 | 1.00 | 14.64 |
| 35 | ATOM | 2297 | CG | GLU | B | 353 | -1.554 | -3.456 | 29.973 | 1.00 | 18.23 |
| | ATOM | 2298 | CD | GLU | B | 353 | -0.620 | -4.355 | 29.176 | 1.00 | 22.72 |
| | ATOM | 2299 | OE1 | GLU | B | 353 | -1.099 | -5.078 | 28.275 | 1.00 | 21.94 |
| | ATOM | 2300 | OE2 | GLU | B | 353 | 0.599 | -4.324 | 29.442 | 1.00 | 24.41 |
| | ATOM | 2301 | C | GLU | B | 353 | -2.729 | 0.119 | 29.219 | 1.00 | 15.85 |
| 40 | ATOM | 2302 | O | GLU | B | 353 | -1.872 | 0.939 | 29.540 | 1.00 | 13.76 |
| | ATOM | 2303 | N | LEU | B | 354 | -3.594 | 0.335 | 28.235 | 1.00 | 12.93 |
| | ATOM | 2304 | CA | LEU | B | 354 | -3.556 | 1.575 | 27.472 | 1.00 | 15.33 |
| | ATOM | 2305 | CB | LEU | B | 354 | -4.616 | 1.534 | 26.360 | 1.00 | 16.44 |
| | ATOM | 2306 | CG | LEU | B | 354 | -4.174 | 0.750 | 25.112 | 1.00 | 17.03 |
| 45 | ATOM | 2307 | CD1 | LEU | B | 354 | -5.373 | 0.509 | 24.189 | 1.00 | 16.70 |
| | ATOM | 2308 | CD2 | LEU | B | 354 | -3.069 | 1.531 | 24.384 | 1.00 | 14.52 |
| | ATOM | 2309 | C | LEU | B | 354 | -3.747 | 2.805 | 28.361 | 1.00 | 12.78 |
| | ATOM | 2310 | O | LEU | B | 354 | -3.123 | 3.850 | 28.141 | 1.00 | 14.28 |
| | ATOM | 2311 | N | VAL | B | 355 | -4.600 | 2.682 | 29.369 | 1.00 | 12.60 |
| 50 | ATOM | 2312 | CA | VAL | B | 355 | -4.844 | 3.791 | 30.279 | 1.00 | 16.78 |
| | ATOM | 2313 | CB | VAL | B | 355 | -5.925 | 3.429 | 31.327 | 1.00 | 16.84 |
| | ATOM | 2314 | CG1 | VAL | B | 355 | -6.070 | 4.561 | 32.344 | 1.00 | 19.88 |
| | ATOM | 2315 | CG2 | VAL | B | 355 | -7.254 | 3.187 | 30.639 | 1.00 | 19.33 |
| | ATOM | 2316 | C | VAL | B | 355 | -3.533 | 4.161 | 30.986 | 1.00 | 19.17 |
| 55 | ATOM | 2317 | O | VAL | B | 355 | -3.158 | 5.328 | 31.049 | 1.00 | 17.30 |
| | ATOM | 2318 | N | HIS | B | 356 | -2.826 | 3.160 | 31.499 | 1.00 | 19.68 |
| | ATOM | 2319 | CA | HIS | B | 356 | -1.559 | 3.418 | 32.177 | 1.00 | 20.64 |
| | ATOM | 2320 | CB | HIS | B | 356 | -1.110 | 2.174 | 32.945 | 1.00 | 21.03 |
| | ATOM | 2321 | CG | HIS | B | 356 | -2.018 | 1.818 | 34.085 | 1.00 | 22.88 |
| 60 | ATOM | 2322 | CD2 | HIS | B | 356 | -3.128 | 1.045 | 34.135 | 1.00 | 21.70 |
| | ATOM | 2323 | ND1 | HIS | B | 356 | -1.838 | 2.312 | 35.358 | 1.00 | 19.24 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 2324 | CE1 | HIS | B | 356 | -2.802 | 1.860 | 36.145 | 1.00 | 18.84 |
| | ATOM | 2325 | NE2 | HIS | B | 356 | -3.598 | 1.088 | 35.426 | 1.00 | 17.92 |
| | ATOM | 2326 | C | HIS | B | 356 | -0.479 | 3.861 | 31.184 | 1.00 | 19.67 |
| | ATOM | 2327 | O | HIS | B | 356 | 0.424 | 4.614 | 31.547 | 1.00 | 19.61 |
| | ATOM | 2328 | N | MET | B | 357 | -0.566 | 3.413 | 29.931 | 1.00 | 14.92 |
| 10 | ATOM | 2329 | CA | MET | B | 357 | 0.428 | 3.830 | 28.939 | 1.00 | 15.13 |
| | ATOM | 2330 | CB | MET | B | 357 | 0.239 | 3.099 | 27.604 | 1.00 | 13.94 |
| | ATOM | 2331 | CG | MET | B | 357 | 1.149 | 3.631 | 26.476 | 1.00 | 14.71 |
| | ATOM | 2332 | SD | MET | B | 357 | 0.747 | 3.014 | 24.826 | 1.00 | 17.75 |
| | ATOM | 2333 | CE | MET | B | 357 | 0.746 | 1.222 | 25.122 | 1.00 | 15.21 |
| 15 | ATOM | 2334 | C | MET | B | 357 | 0.316 | 5.334 | 28.699 | 1.00 | 14.94 |
| | ATOM | 2335 | O | MET | B | 357 | 1.319 | 6.031 | 28.560 | 1.00 | 17.02 |
| | ATOM | 2336 | N | ILE | B | 358 | -0.909 | 5.839 | 28.659 | 1.00 | 18.01 |
| | ATOM | 2337 | CA | ILE | B | 358 | -1.122 | 7.263 | 28.423 | 1.00 | 19.77 |
| | ATOM | 2338 | CB | ILE | B | 358 | -2.634 | 7.577 | 28.287 | 1.00 | 23.11 |
| 20 | ATOM | 2339 | CG2 | ILE | B | 358 | -2.879 | 9.080 | 28.450 | 1.00 | 25.00 |
| | ATOM | 2340 | CG1 | ILE | B | 358 | -3.137 | 7.105 | 26.913 | 1.00 | 24.19 |
| | ATOM | 2341 | CD1 | ILE | B | 358 | -4.600 | 6.653 | 26.890 | 1.00 | 20.17 |
| | ATOM | 2342 | C | ILE | B | 358 | -0.501 | 8.100 | 29.550 | 1.00 | 22.93 |
| | ATOM | 2343 | O | ILE | B | 358 | 0.080 | 9.153 | 29.299 | 1.00 | 23.33 |
| 25 | ATOM | 2344 | N | ASN | B | 359 | -0.619 | 7.631 | 30.790 | 1.00 | 22.34 |
| | ATOM | 2345 | CA | ASN | B | 359 | -0.029 | 8.341 | 31.924 | 1.00 | 23.24 |
| | ATOM | 2346 | CB | ASN | B | 359 | -0.480 | 7.726 | 33.224 | 1.00 | 25.10 |
| | ATOM | 2347 | CG | ASN | B | 359 | -1.831 | 8.171 | 33.649 | 1.00 | 32.65 |
| | ATOM | 2348 | OD1 | ASN | B | 359 | -2.421 | 9.069 | 33.042 | 1.00 | 32.98 |
| 30 | ATOM | 2349 | ND2 | ASN | B | 359 | -2.364 | 7.549 | 34.691 | 1.00 | 33.87 |
| | ATOM | 2350 | C | ASN | B | 359 | 1.473 | 8.306 | 31.837 | 1.00 | 24.77 |
| | ATOM | 2351 | O | ASN | B | 359 | 2.152 | 9.285 | 32.149 | 1.00 | 24.19 |
| | ATOM | 2352 | N | TRP | B | 360 | 1.995 | 7.149 | 31.438 | 1.00 | 20.82 |
| | ATOM | 2353 | CA | TRP | B | 360 | 3.439 | 6.965 | 31.310 | 1.00 | 19.29 |
| 35 | ATOM | 2354 | CB | TRP | B | 360 | 3.754 | 5.524 | 30.878 | 1.00 | 18.59 |
| | ATOM | 2355 | CG | TRP | B | 360 | 5.085 | 5.363 | 30.176 | 1.00 | 18.21 |
| | ATOM | 2356 | CD2 | TRP | B | 360 | 5.310 | 5.308 | 28.756 | 1.00 | 14.38 |
| | ATOM | 2357 | CE2 | TRP | B | 360 | 6.698 | 5.129 | 28.561 | 1.00 | 13.42 |
| | ATOM | 2358 | CE3 | TRP | B | 360 | 4.475 | 5.392 | 27.633 | 1.00 | 15.52 |
| 40 | ATOM | 2359 | CD1 | TRP | B | 360 | 6.306 | 5.221 | 30.762 | 1.00 | 13.34 |
| | ATOM | 2360 | NE1 | TRP | B | 360 | 7.283 | 5.078 | 29.800 | 1.00 | 16.05 |
| | ATOM | 2361 | CZ2 | TRP | B | 360 | 7.272 | 5.032 | 27.288 | 1.00 | 16.84 |
| | ATOM | 2362 | CZ3 | TRP | B | 360 | 5.045 | 5.296 | 26.363 | 1.00 | 15.11 |
| | ATOM | 2363 | CH2 | TRP | B | 360 | 6.431 | 5.115 | 26.202 | 1.00 | 16.12 |
| 45 | ATOM | 2364 | C | TRP | B | 360 | 3.979 | 7.939 | 30.273 | 1.00 | 20.13 |
| | ATOM | 2365 | O | TRP | B | 360 | 4.991 | 8.606 | 30.497 | 1.00 | 17.26 |
| | ATOM | 2366 | N | ALA | B | 361 | 3.295 | 8.012 | 29.135 | 1.00 | 19.34 |
| | ATOM | 2367 | CA | ALA | B | 361 | 3.708 | 8.900 | 28.051 | 1.00 | 22.01 |
| | ATOM | 2368 | CB | ALA | B | 361 | 2.682 | 8.855 | 26.921 | 1.00 | 19.53 |
| 50 | ATOM | 2369 | C | ALA | B | 361 | 3.883 | 10.336 | 28.552 | 1.00 | 22.39 |
| | ATOM | 2370 | O | ALA | B | 361 | 4.858 | 11.005 | 28.210 | 1.00 | 19.57 |
| | ATOM | 2371 | N | LYS | B | 362 | 2.932 | 10.794 | 29.361 | 1.00 | 21.96 |
| | ATOM | 2372 | CA | LYS | B | 362 | 2.966 | 12.139 | 29.923 | 1.00 | 26.45 |
| | ATOM | 2373 | CB | LYS | B | 362 | 1.741 | 12.363 | 30.811 | 1.00 | 29.79 |
| 55 | ATOM | 2374 | CG | LYS | B | 362 | 0.426 | 12.417 | 30.064 | 1.00 | 33.57 |
| | ATOM | 2375 | CD | LYS | B | 362 | -0.563 | 13.304 | 30.805 | 1.00 | 36.83 |
| | ATOM | 2376 | CE | LYS | B | 362 | -1.620 | 12.490 | 31.512 | 1.00 | 36.89 |
| | ATOM | 2377 | NZ | LYS | B | 362 | -2.873 | 13.276 | 31.664 | 1.00 | 39.07 |
| | ATOM | 2378 | C | LYS | B | 362 | 4.223 | 12.379 | 30.757 | 1.00 | 27.77 |
| 60 | ATOM | 2379 | O | LYS | B | 362 | 4.661 | 13.517 | 30.922 | 1.00 | 26.93 |
| | ATOM | 2380 | N | ARG | B | 363 | 4.805 | 11.302 | 31.278 | 1.00 | 26.61 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 2381 | CA | ARG | B | 363 | 5.996 | 11.414 | 32.109 | 1.00 | 27.74 |
| | ATOM | 2382 | CB | ARG | B | 363 | 5.887 | 10.457 | 33.298 | 1.00 | 28.93 |
| | ATOM | 2383 | CG | ARG | B | 363 | 4.650 | 10.704 | 34.158 | 1.00 | 36.07 |
| | ATOM | 2384 | CD | ARG | B | 363 | 4.569 | 9.745 | 35.344 | 1.00 | 42.83 |
| | ATOM | 2385 | NE | ARG | B | 363 | 4.477 | 8.344 | 34.928 | 1.00 | 49.79 |
| 10 | ATOM | 2386 | CZ | ARG | B | 363 | 3.395 | 7.582 | 35.080 | 1.00 | 51.48 |
| | ATOM | 2387 | NH1 | ARG | B | 363 | 2.300 | 8.081 | 35.648 | 1.00 | 52.17 |
| | ATOM | 2388 | NH2 | ARG | B | 363 | 3.405 | 6.316 | 34.668 | 1.00 | 40.24 |
| | ATOM | 2389 | C | ARG | B | 363 | 7.308 | 11.190 | 31.367 | 1.00 | 25.80 |
| | ATOM | 2390 | O | ARG | B | 363 | 8.374 | 11.183 | 31.975 | 1.00 | 29.36 |
| 15 | ATOM | 2391 | N | VAL | B | 364 | 7.231 | 11.009 | 30.053 | 1.00 | 24.28 |
| | ATOM | 2392 | CA | VAL | B | 364 | 8.431 | 10.823 | 29.248 | 1.00 | 21.87 |
| | ATOM | 2393 | CB | VAL | B | 364 | 8.116 | 10.048 | 27.947 | 1.00 | 21.84 |
| | ATOM | 2394 | CG1 | VAL | B | 364 | 9.267 | 10.184 | 26.968 | 1.00 | 15.85 |
| | ATOM | 2395 | CG2 | VAL | B | 364 | 7.860 | 8.560 | 28.268 | 1.00 | 16.24 |
| 20 | ATOM | 2396 | C | VAL | B | 364 | 8.925 | 12.241 | 28.923 | 1.00 | 28.14 |
| | ATOM | 2397 | O | VAL | B | 364 | 8.219 | 13.023 | 28.285 | 1.00 | 24.24 |
| | ATOM | 2398 | N | PRO | B | 365 | 10.141 | 12.591 | 29.375 | 1.00 | 28.57 |
| | ATOM | 2399 | CD | PRO | B | 365 | 11.061 | 11.726 | 30.137 | 1.00 | 30.58 |
| | ATOM | 2400 | CA | PRO | B | 365 | 10.719 | 13.919 | 29.138 | 1.00 | 32.16 |
| 25 | ATOM | 2401 | CB | PRO | B | 365 | 12.189 | 13.739 | 29.507 | 1.00 | 32.70 |
| | ATOM | 2402 | CG | PRO | B | 365 | 12.170 | 12.671 | 30.545 | 1.00 | 33.35 |
| | ATOM | 2403 | C | PRO | B | 365 | 10.546 | 14.464 | 27.726 | 1.00 | 32.22 |
| | ATOM | 2404 | O | PRO | B | 365 | 11.056 | 13.897 | 26.766 | 1.00 | 37.04 |
| | ATOM | 2405 | N | GLY | B | 366 | 9.821 | 15.570 | 27.609 | 1.00 | 34.09 |
| 30 | ATOM | 2406 | CA | GLY | B | 366 | 9.612 | 16.182 | 26.310 | 1.00 | 32.54 |
| | ATOM | 2407 | C | GLY | B | 366 | 8.241 | 15.969 | 25.700 | 1.00 | 33.46 |
| | ATOM | 2408 | O | GLY | B | 366 | 7.791 | 16.779 | 24.886 | 1.00 | 33.73 |
| | ATOM | 2409 | N | PHE | B | 367 | 7.564 | 14.895 | 26.096 | 1.00 | 31.08 |
| | ATOM | 2410 | CA | PHE | B | 367 | 6.250 | 14.593 | 25.542 | 1.00 | 28.60 |
| 35 | ATOM | 2411 | CB | PHE | B | 367 | 5.745 | 13.244 | 26.058 | 1.00 | 25.96 |
| | ATOM | 2412 | CG | PHE | B | 367 | 4.629 | 12.671 | 25.239 | 1.00 | 22.75 |
| | ATOM | 2413 | CD1 | PHE | B | 367 | 3.313 | 12.771 | 25.669 | 1.00 | 22.62 |
| | ATOM | 2414 | CD2 | PHE | B | 367 | 4.897 | 12.025 | 24.033 | 1.00 | 22.29 |
| | ATOM | 2415 | CE1 | PHE | B | 367 | 2.272 | 12.233 | 24.914 | 1.00 | 25.63 |
| 40 | ATOM | 2416 | CE2 | PHE | B | 367 | 3.867 | 11.486 | 23.272 | 1.00 | 20.82 |
| | ATOM | 2417 | CZ | PHE | B | 367 | 2.553 | 11.588 | 23.711 | 1.00 | 25.50 |
| | ATOM | 2418 | C | PHE | B | 367 | 5.178 | 15.646 | 25.781 | 1.00 | 26.79 |
| | ATOM | 2419 | O | PHE | B | 367 | 4.458 | 16.001 | 24.854 | 1.00 | 23.37 |
| | ATOM | 2420 | N | VAL | B | 368 | 5.049 | 16.143 | 27.009 | 1.00 | 31.26 |
| 45 | ATOM | 2421 | CA | VAL | B | 368 | 4.020 | 17.151 | 27.277 | 1.00 | 35.71 |
| | ATOM | 2422 | CB | VAL | B | 368 | 3.817 | 17.412 | 28.795 | 1.00 | 35.98 |
| | ATOM | 2423 | CG1 | VAL | B | 368 | 2.944 | 16.320 | 29.392 | 1.00 | 37.64 |
| | ATOM | 2424 | CG2 | VAL | B | 368 | 5.157 | 17.495 | 29.508 | 1.00 | 35.81 |
| | ATOM | 2425 | C | VAL | B | 368 | 4.328 | 18.482 | 26.598 | 1.00 | 35.87 |
| 50 | ATOM | 2426 | O | VAL | B | 368 | 3.450 | 19.330 | 26.457 | 1.00 | 37.71 |
| | ATOM | 2427 | N | ASP | B | 369 | 5.572 | 18.665 | 26.175 | 1.00 | 35.49 |
| | ATOM | 2428 | CA | ASP | B | 369 | 5.950 | 19.904 | 25.503 | 1.00 | 36.54 |
| | ATOM | 2429 | CB | ASP | B | 369 | 7.466 | 19.963 | 25.309 | 1.00 | 39.79 |
| | ATOM | 2430 | CG | ASP | B | 369 | 8.213 | 20.169 | 26.615 | 1.00 | 44.33 |
| 55 | ATOM | 2431 | OD1 | ASP | B | 369 | 9.409 | 19.807 | 26.684 | 1.00 | 48.45 |
| | ATOM | 2432 | OD2 | ASP | B | 369 | 7.604 | 20.693 | 27.572 | 1.00 | 43.27 |
| | ATOM | 2433 | C | ASP | B | 369 | 5.248 | 19.997 | 24.149 | 1.00 | 34.49 |
| | ATOM | 2434 | O | ASP | B | 369 | 5.131 | 21.074 | 23.571 | 1.00 | 34.51 |
| | ATOM | 2435 | N | LEU | B | 370 | 4.776 | 18.859 | 23.653 | 1.00 | 30.97 |
| 60 | ATOM | 2436 | CA | LEU | B | 370 | 4.086 | 18.809 | 22.370 | 1.00 | 29.80 |
| | ATOM | 2437 | CB | LEU | B | 370 | 4.145 | 17.389 | 21.799 | 1.00 | 27.27 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 2438 | CG | LEU | B | 370 | 5.522 | 16.733 | 21.688 | 1.00 | 28.07 |
| | ATOM | 2439 | CD1 | LEU | B | 370 | 5.353 | 15.242 | 21.400 | 1.00 | 30.38 |
| | ATOM | 2440 | CD2 | LEU | B | 370 | 6.316 | 17.396 | 20.574 | 1.00 | 22.82 |
| | ATOM | 2441 | C | LEU | B | 370 | 2.628 | 19.218 | 22.521 | 1.00 | 28.04 |
| | ATOM | 2442 | O | LEU | B | 370 | 2.066 | 19.151 | 23.611 | 1.00 | 29.71 |
| 10 | ATOM | 2443 | N | THR | B | 371 | 2.011 | 19.645 | 21.425 | 1.00 | 28.70 |
| | ATOM | 2444 | CA | THR | B | 371 | 0.602 | 20.014 | 21.474 | 1.00 | 30.31 |
| | ATOM | 2445 | CB | THR | B | 371 | 0.150 | 20.690 | 20.163 | 1.00 | 31.96 |
| | ATOM | 2446 | OG1 | THR | B | 371 | 0.284 | 19.763 | 19.080 | 1.00 | 29.49 |
| | ATOM | 2447 | CG2 | THR | B | 371 | 0.991 | 21.930 | 19.878 | 1.00 | 29.98 |
| 15 | ATOM | 2448 | C | THR | B | 371 | -0.208 | 18.726 | 21.666 | 1.00 | 30.59 |
| | ATOM | 2449 | O | THR | B | 371 | 0.300 | 17.624 | 21.431 | 1.00 | 27.10 |
| | ATOM | 2450 | N | LEU | B | 372 | -1.461 | 18.863 | 22.087 | 1.00 | 27.65 |
| | ATOM | 2451 | CA | LEU | B | 372 | -2.323 | 17.702 | 22.303 | 1.00 | 30.86 |
| | ATOM | 2452 | CB | LEU | B | 372 | -3.722 | 18.147 | 22.737 | 1.00 | 30.11 |
| 20 | ATOM | 2453 | CG | LEU | B | 372 | -4.715 | 17.006 | 22.960 | 1.00 | 32.80 |
| | ATOM | 2454 | CD1 | LEU | B | 372 | -4.231 | 16.147 | 24.126 | 1.00 | 34.10 |
| | ATOM | 2455 | CD2 | LEU | B | 372 | -6.105 | 17.562 | 23.246 | 1.00 | 31.16 |
| | ATOM | 2456 | C | LEU | B | 372 | -2.437 | 16.863 | 21.034 | 1.00 | 31.77 |
| | ATOM | 2457 | O | LEU | B | 372 | -2.417 | 15.629 | 21.078 | 1.00 | 27.06 |
| 25 | ATOM | 2458 | N | HIS | B | 373 | -2.564 | 17.548 | 19.905 | 1.00 | 31.30 |
| | ATOM | 2459 | CA | HIS | B | 373 | -2.685 | 16.888 | 18.614 | 1.00 | 31.35 |
| | ATOM | 2460 | CB | HIS | B | 373 | -2.844 | 17.935 | 17.503 | 1.00 | 34.30 |
| | ATOM | 2461 | CG | HIS | B | 373 | -2.503 | 17.430 | 16.132 | 1.00 | 41.27 |
| | ATOM | 2462 | CD2 | HIS | B | 373 | -3.293 | 17.105 | 15.079 | 1.00 | 42.50 |
| 30 | ATOM | 2463 | ND1 | HIS | B | 373 | -1.205 | 17.220 | 15.715 | 1.00 | 43.69 |
| | ATOM | 2464 | CE1 | HIS | B | 373 | -1.210 | 16.787 | 14.465 | 1.00 | 48.87 |
| | ATOM | 2465 | NE2 | HIS | B | 373 | -2.465 | 16.708 | 14.056 | 1.00 | 43.72 |
| | ATOM | 2466 | C | HIS | B | 373 | -1.468 | 16.012 | 18.337 | 1.00 | 28.29 |
| | ATOM | 2467 | O | HIS | B | 373 | -1.610 | 14.878 | 17.897 | 1.00 | 30.21 |
| 35 | ATOM | 2468 | N | ASP | B | 374 | -0.275 | 16.541 | 18.589 | 1.00 | 28.85 |
| | ATOM | 2469 | CA | ASP | B | 374 | 0.950 | 15.783 | 18.350 | 1.00 | 28.28 |
| | ATOM | 2470 | CB | ASP | B | 374 | 2.178 | 16.678 | 18.535 | 1.00 | 31.33 |
| | ATOM | 2471 | CG | ASP | B | 374 | 2.433 | 17.577 | 17.333 | 1.00 | 39.07 |
| | ATOM | 2472 | OD1 | ASP | B | 374 | 3.195 | 18.557 | 17.478 | 1.00 | 40.60 |
| 40 | ATOM | 2473 | OD2 | ASP | B | 374 | 1.874 | 17.305 | 16.246 | 1.00 | 38.64 |
| | ATOM | 2474 | C | ASP | B | 374 | 1.029 | 14.592 | 19.303 | 1.00 | 29.05 |
| | ATOM | 2475 | O | ASP | B | 374 | 1.432 | 13.494 | 18.908 | 1.00 | 24.26 |
| | ATOM | 2476 | N | GLN | B | 375 | 0.642 | 14.814 | 20.556 | 1.00 | 24.52 |
| | ATOM | 2477 | CA | GLN | B | 375 | 0.667 | 13.749 | 21.547 | 1.00 | 27.37 |
| 45 | ATOM | 2478 | CB | GLN | B | 375 | 0.213 | 14.270 | 22.901 | 1.00 | 26.66 |
| | ATOM | 2479 | CG | GLN | B | 375 | 1.164 | 15.236 | 23.563 | 1.00 | 29.74 |
| | ATOM | 2480 | CD | GLN | B | 375 | 0.623 | 15.691 | 24.890 | 1.00 | 33.13 |
| | ATOM | 2481 | OE1 | GLN | B | 375 | -0.044 | 14.953 | 25.602 | 1.00 | 32.82 |
| | ATOM | 2482 | NE2 | GLN | B | 375 | 0.895 | 16.953 | 25.236 | 1.00 | 33.98 |
| 50 | ATOM | 2483 | C | GLN | B | 375 | -0.259 | 12.630 | 21.104 | 1.00 | 24.52 |
| | ATOM | 2484 | O | GLN | B | 375 | 0.074 | 11.451 | 21.221 | 1.00 | 23.56 |
| | ATOM | 2485 | N | VAL | B | 376 | -1.426 | 13.013 | 20.599 | 1.00 | 21.87 |
| | ATOM | 2486 | CA | VAL | B | 376 | -2.409 | 12.055 | 20.140 | 1.00 | 23.44 |
| | ATOM | 2487 | CB | VAL | B | 376 | -3.718 | 12.760 | 19.717 | 1.00 | 22.09 |
| 55 | ATOM | 2488 | CG1 | VAL | B | 376 | -4.572 | 11.823 | 18.877 | 1.00 | 24.14 |
| | ATOM | 2489 | CG2 | VAL | B | 376 | -4.486 | 13.192 | 20.954 | 1.00 | 16.96 |
| | ATOM | 2490 | C | VAL | B | 376 | -1.852 | 11.257 | 18.965 | 1.00 | 24.15 |
| | ATOM | 2491 | O | VAL | B | 376 | -1.949 | 10.032 | 18.938 | 1.00 | 22.26 |
| | ATOM | 2492 | N | HIS | B | 377 | -1.251 | 11.953 | 18.007 | 1.00 | 25.85 |
| 60 | ATOM | 2493 | CA | HIS | B | 377 | -0.689 | 11.284 | 16.843 | 1.00 | 25.68 |
| | ATOM | 2494 | CB | HIS | B | 377 | -0.078 | 12.306 | 15.886 | 1.00 | 25.27 |

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|----|------|------|-----|------|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 2495 | CG | HIS | B | 377 | 0.535 | 11.690 | 14.667 | 1.00 | 30.63 |
| | ATOM | 2496 | CD2 | HIS | B | 377 | 1.828 | 11.559 | 14.287 | 1.00 | 31.03 |
| | ATOM | 2497 | ND1 | HIS | B | 377 | -0.217 | 11.086 | 13.683 | 1.00 | 35.05 |
| | ATOM | 2498 | CE1 | HIS | B | 377 | 0.588 | 10.607 | 12.750 | 1.00 | 33.12 |
| | ATOM | 2499 | NE2 | HIS | B | 377 | 1.833 | 10.882 | 13.093 | 1.00 | 31.06 |
| 10 | ATOM | 2500 | C | HIS | B | 377 | 0.365 | 10.237 | 17.210 | 1.00 | 24.37 |
| | ATOM | 2501 | O | HIS | B | 377 | 0.321 | 9.109 | 16.719 | 1.00 | 21.47 |
| | ATOM | 2502 | N | LEU | B | 378 | 1.307 | 10.609 | 18.072 | 1.00 | 19.24 |
| | ATOM | 2503 | CA | LEU | B | 378 | 2.365 | 9.691 | 18.474 | 1.00 | 20.09 |
| | ATOM | 2504 | CB | LEU | B | 378 | 3.363 | 10.402 | 19.388 | 1.00 | 18.64 |
| 15 | ATOM | 2505 | CG | LEU | B | 378 | 4.230 | 11.489 | 18.736 | 1.00 | 22.15 |
| | ATOM | 2506 | CD1 | LEU | B | 378 | 5.104 | 12.148 | 19.796 | 1.00 | 22.51 |
| | ATOM | 2507 | CD2 | LEU | B | 378 | 5.094 | 10.885 | 17.638 | 1.00 | 20.68 |
| | ATOM | 2508 | C | LEU | B | 378 | 1.832 | 8.433 | 19.161 | 1.00 | 18.91 |
| | ATOM | 2509 | O | LEU | B | 378 | 2.262 | 7.320 | 18.859 | 1.00 | 17.52 |
| 20 | ATOM | 2510 | N | LEU | B | 379 | 0.888 | 8.610 | 20.077 | 1.00 | 18.25 |
| | ATOM | 2511 | CA | LEU | B | 379 | 0.317 | 7.486 | 20.795 | 1.00 | 18.60 |
| | ATOM | 2512 | CB | LEU | B | 379 | -0.526 | 7.989 | 21.968 | 1.00 | 16.77 |
| | ATOM | 2513 | CG | LEU | B | 379 | 0.292 | 8.353 | 23.214 | 1.00 | 17.90 |
| | ATOM | 2514 | CD1 | LEU | B | 379 | -0.578 | 9.092 | 24.211 | 1.00 | 15.84 |
| 25 | ATOM | 2515 | CD2 | LEU | B | 379 | 0.851 | 7.075 | 23.842 | 1.00 | 22.09 |
| | ATOM | 2516 | C | LEU | B | 379 | -0.518 | 6.605 | 19.872 | 1.00 | 20.17 |
| | ATOM | 2517 | O | LEU | B | 379 | -0.476 | 5.377 | 19.968 | 1.00 | 18.11 |
| | ATOM | 2518 | N | GLU | B | 380 | -1.273 | 7.222 | 18.971 | 1.00 | 19.40 |
| | ATOM | 2519 | CA | GLU | B | 380 | -2.086 | 6.435 | 18.049 | 1.00 | 20.19 |
| 30 | ATOM | 2520 | CB | GLU | B | 380 | -2.994 | 7.350 | 17.222 | 1.00 | 22.43 |
| | ATOM | 2521 | CG | GLU | B | 380 | -4.182 | 7.874 | 18.007 | 1.00 | 25.30 |
| | ATOM | 2522 | CD | GLU | B | 380 | -5.070 | 8.789 | 17.188 | 1.00 | 29.44 |
| | ATOM | 2523 | OE1 | GLU | B | 380 | -6.206 | 9.066 | 17.625 | 1.00 | 31.70 |
| | ATOM | 2524 | OE2 | GLU | B | 380 | -4.631 | 9.230 | 16.110 | 1.00 | 31.75 |
| 35 | ATOM | 2525 | C | GLU | B | 380 | -1.210 | 5.594 | 17.117 | 1.00 | 18.92 |
| | ATOM | 2526 | O | GLU | B | 380 | -1.586 | 4.491 | 16.722 | 1.00 | 19.83 |
| | ATOM | 2527 | N | ACYS | B | 381 | -0.039 | 6.113 | 16.772 | 0.75 | 17.41 |
| | ATOM | 2528 | N | BCYS | B | 381 | -0.035 | 6.113 | 16.779 | 0.25 | 17.76 |
| | ATOM | 2529 | CA | ACYS | B | 381 | 0.860 | 5.384 | 15.887 | 0.75 | 20.19 |
| 40 | ATOM | 2530 | CA | BCYS | B | 381 | 0.875 | 5.407 | 15.884 | 0.25 | 17.50 |
| | ATOM | 2531 | CB | ACYS | B | 381 | 1.870 | 6.342 | 15.248 | 0.75 | 24.20 |
| | ATOM | 2532 | CB | BCYS | B | 381 | 1.830 | 6.406 | 15.226 | 0.25 | 16.63 |
| | ATOM | 2533 | SG | ACYS | B | 381 | 1.167 | 7.518 | 14.060 | 0.75 | 33.54 |
| | ATOM | 2534 | SG | BCYS | B | 381 | 3.048 | 5.656 | 14.128 | 0.25 | 10.36 |
| 45 | ATOM | 2535 | C | ACYS | B | 381 | 1.626 | 4.269 | 16.592 | 0.75 | 20.59 |
| | ATOM | 2536 | C | BCYS | B | 381 | 1.689 | 4.305 | 16.561 | 0.25 | 19.19 |
| | ATOM | 2537 | O | ACYS | B | 381 | 1.737 | 3.161 | 16.069 | 0.75 | 19.16 |
| | ATOM | 2538 | O | BCYS | B | 381 | 1.904 | 3.241 | 15.982 | 0.25 | 19.25 |
| | ATOM | 2539 | N | ALA | B | 382 | 2.134 | 4.560 | 17.785 | 1.00 | 19.04 |
| 50 | ATOM | 2540 | CA | ALA | B | 382 | 2.955 | 3.602 | 18.530 | 1.00 | 20.27 |
| | ATOM | 2541 | CB | ALA | B | 382 | 4.135 | 4.364 | 19.143 | 1.00 | 18.68 |
| | ATOM | 2542 | C | ALA | B | 382 | 2.356 | 2.702 | 19.607 | 1.00 | 16.82 |
| | ATOM | 2543 | O | ALA | B | 382 | 3.070 | 1.852 | 20.142 | 1.00 | 13.37 |
| | ATOM | 2544 | N | TRP | B | 383 | 1.074 | 2.855 | 19.916 | 1.00 | 15.30 |
| 55 | ATOM | 2545 | CA | TRP | B | 383 | 0.487 | 2.089 | 21.013 | 1.00 | 15.80 |
| | ATOM | 2546 | CB | TRP | B | 383 | -1.009 | 2.410 | 21.160 | 1.00 | 16.63 |
| | ATOM | 2547 | CG | TRP | B | 383 | -1.871 | 1.775 | 20.129 | 1.00 | 19.93 |
| | ATOM | 2548 | CD2 | TRP | B | 383 | -2.493 | 0.483 | 20.198 | 1.00 | 20.80 |
| | ATOM | 2549 | CE2 | TRP | B | 383 | -3.226 | 0.309 | 19.003 | 1.00 | 19.27 |
| 60 | ATOM | 2550 | CE3 | TRP | B | 383 | -2.506 | -0.542 | 21.155 | 1.00 | 21.32 |
| | ATOM | 2551 | CD1 | TRP | B | 383 | -2.236 | 2.312 | 18.933 | 1.00 | 18.59 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 2552 | NE1 | TRP | B | 383 | -3.051 | 1.439 | 18.250 | 1.00 | 23.67 |
| | ATOM | 2553 | CZ2 | TRP | B | 383 | -3.963 | -0.853 | 18.733 | 1.00 | 21.55 |
| | ATOM | 2554 | CZ3 | TRP | B | 383 | -3.243 | -1.702 | 20.888 | 1.00 | 20.29 |
| | ATOM | 2555 | CH2 | TRP | B | 383 | -3.960 | -1.844 | 19.686 | 1.00 | 19.03 |
| | ATOM | 2556 | C | TRP | B | 383 | 0.701 | 0.579 | 21.020 | 1.00 | 17.35 |
| 10 | ATOM | 2557 | O | TRP | B | 383 | 0.982 | 0.010 | 22.077 | 1.00 | 13.92 |
| | ATOM | 2558 | N | LEU | B | 384 | 0.568 | -0.087 | 19.879 | 1.00 | 14.07 |
| | ATOM | 2559 | CA | LEU | B | 384 | 0.773 | -1.532 | 19.903 | 1.00 | 15.98 |
| | ATOM | 2560 | CB | LEU | B | 384 | 0.181 | -2.200 | 18.656 | 1.00 | 12.19 |
| | ATOM | 2561 | CG | LEU | B | 384 | 0.173 | -3.735 | 18.720 | 1.00 | 12.97 |
| 15 | ATOM | 2562 | CD1 | LEU | B | 384 | -0.352 | -4.240 | 20.089 | 1.00 | 10.65 |
| | ATOM | 2563 | CD2 | LEU | B | 384 | -0.707 | -4.259 | 17.586 | 1.00 | 17.84 |
| | ATOM | 2564 | C | LEU | B | 384 | 2.262 | -1.861 | 20.034 | 1.00 | 14.64 |
| | ATOM | 2565 | O | LEU | B | 384 | 2.627 | -2.833 | 20.690 | 1.00 | 13.78 |
| | ATOM | 2566 | N | GLU | B | 385 | 3.116 | -1.046 | 19.414 | 1.00 | 14.96 |
| 20 | ATOM | 2567 | CA | GLU | B | 385 | 4.565 | -1.260 | 19.509 | 1.00 | 13.79 |
| | ATOM | 2568 | CB | GLU | B | 385 | 5.336 | -0.179 | 18.739 | 1.00 | 15.34 |
| | ATOM | 2569 | CG | GLU | B | 385 | 5.297 | -0.312 | 17.207 | 1.00 | 15.38 |
| | ATOM | 2570 | CD | GLU | B | 385 | 6.162 | 0.738 | 16.520 | 1.00 | 23.97 |
| | ATOM | 2571 | OE1 | GLU | B | 385 | 7.381 | 0.500 | 16.358 | 1.00 | 21.03 |
| 25 | ATOM | 2572 | OE2 | GLU | B | 385 | 5.622 | 1.808 | 16.149 | 1.00 | 22.19 |
| | ATOM | 2573 | C | GLU | B | 385 | 4.963 | -1.161 | 20.987 | 1.00 | 15.79 |
| | ATOM | 2574 | O | GLU | B | 385 | 5.788 | -1.942 | 21.463 | 1.00 | 15.04 |
| | ATOM | 2575 | N | ILE | B | 386 | 4.389 | -0.213 | 21.690 | 1.00 | 13.32 |
| | ATOM | 2576 | CA | ILE | B | 386 | 4.723 | -0.019 | 23.108 | 1.00 | 14.06 |
| 30 | ATOM | 2577 | CB | ILE | B | 386 | 4.173 | 1.326 | 23.614 | 1.00 | 15.36 |
| | ATOM | 2578 | CG2 | ILE | B | 386 | 4.374 | 1.451 | 25.130 | 1.00 | 15.97 |
| | ATOM | 2579 | CG1 | ILE | B | 386 | 4.910 | 2.476 | 22.907 | 1.00 | 17.95 |
| | ATOM | 2580 | CD1 | ILE | B | 386 | 4.118 | 3.768 | 22.874 | 1.00 | 21.12 |
| | ATOM | 2581 | C | ILE | B | 386 | 4.227 | -1.164 | 23.993 | 1.00 | 14.97 |
| 35 | ATOM | 2582 | O | ILE | B | 386 | 4.905 | -1.560 | 24.941 | 1.00 | 19.60 |
| | ATOM | 2583 | N | LEU | B | 387 | 3.038 | -1.675 | 23.709 | 1.00 | 15.18 |
| | ATOM | 2584 | CA | LEU | B | 387 | 2.516 | -2.791 | 24.478 | 1.00 | 15.98 |
| | ATOM | 2585 | CB | LEU | B | 387 | 1.070 | -3.097 | 24.080 | 1.00 | 17.15 |
| | ATOM | 2586 | CG | LEU | B | 387 | -0.031 | -2.113 | 24.486 | 1.00 | 19.65 |
| 40 | ATOM | 2587 | CD1 | LEU | B | 387 | -1.371 | -2.628 | 23.972 | 1.00 | 17.77 |
| | ATOM | 2588 | CD2 | LEU | B | 387 | -0.075 | -1.966 | 26.002 | 1.00 | 15.38 |
| | ATOM | 2589 | C | LEU | B | 387 | 3.391 | -4.013 | 24.180 | 1.00 | 14.69 |
| | ATOM | 2590 | O | LEU | B | 387 | 3.712 | -4.792 | 25.076 | 1.00 | 14.03 |
| | ATOM | 2591 | N | MET | B | 388 | 3.785 | -4.178 | 22.921 | 1.00 | 16.43 |
| 45 | ATOM | 2592 | CA | MET | B | 388 | 4.602 | -5.329 | 22.547 | 1.00 | 16.67 |
| | ATOM | 2593 | CB | MET | B | 388 | 4.673 | -5.460 | 21.026 | 1.00 | 14.83 |
| | ATOM | 2594 | CG | MET | B | 388 | 3.403 | -6.066 | 20.453 | 1.00 | 13.91 |
| | ATOM | 2595 | SD | MET | B | 388 | 3.364 | -6.193 | 18.675 | 1.00 | 17.23 |
| | ATOM | 2596 | CE | MET | B | 388 | 1.906 | -7.225 | 18.511 | 1.00 | 14.97 |
| 50 | ATOM | 2597 | C | MET | B | 388 | 6.004 | -5.332 | 23.133 | 1.00 | 20.19 |
| | ATOM | 2598 | O | MET | B | 388 | 6.460 | -6.366 | 23.636 | 1.00 | 21.50 |
| | ATOM | 2599 | N | ILE | B | 389 | 6.707 | -4.203 | 23.074 | 1.00 | 15.34 |
| | ATOM | 2600 | CA | ILE | B | 389 | 8.044 | -4.209 | 23.634 | 1.00 | 15.59 |
| | ATOM | 2601 | CB | ILE | B | 389 | 8.836 | -2.911 | 23.322 | 1.00 | 14.95 |
| 55 | ATOM | 2602 | CG2 | ILE | B | 389 | 8.330 | -1.746 | 24.158 | 1.00 | 12.81 |
| | ATOM | 2603 | CG1 | ILE | B | 389 | 10.325 | -3.164 | 23.602 | 1.00 | 17.24 |
| | ATOM | 2604 | CD1 | ILE | B | 389 | 11.228 | -1.972 | 23.357 | 1.00 | 15.65 |
| | ATOM | 2605 | C | ILE | B | 389 | 7.950 | -4.446 | 25.147 | 1.00 | 14.30 |
| | ATOM | 2606 | O | ILE | B | 389 | 8.844 | -5.044 | 25.739 | 1.00 | 18.72 |
| 60 | ATOM | 2607 | N | GLY | B | 390 | 6.855 | -4.007 | 25.761 | 1.00 | 13.99 |
| | ATOM | 2608 | CA | GLY | B | 390 | 6.681 | -4.219 | 27.189 | 1.00 | 14.87 |

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 2609 | C | GLY | B | 390 | 6.444 | -5.702 | 27.463 | 1.00 | 18.54 |
| | ATOM | 2610 | O | GLY | B | 390 | 6.989 | -6.282 | 28.403 | 1.00 | 16.54 |
| | ATOM | 2611 | N | LEU | B | 391 | 5.623 | -6.325 | 26.628 | 1.00 | 16.15 |
| | ATOM | 2612 | CA | LEU | B | 391 | 5.334 | -7.743 | 26.775 | 1.00 | 18.91 |
| | ATOM | 2613 | CB | LEU | B | 391 | 4.332 | -8.179 | 25.699 | 1.00 | 19.55 |
| 10 | ATOM | 2614 | CG | LEU | B | 391 | 4.157 | -9.689 | 25.457 | 1.00 | 20.91 |
| | ATOM | 2615 | CD1 | LEU | B | 391 | 3.580 | -10.351 | 26.699 | 1.00 | 19.41 |
| | ATOM | 2616 | CD2 | LEU | B | 391 | 3.232 | -9.913 | 24.268 | 1.00 | 20.70 |
| | ATOM | 2617 | C | LEU | B | 391 | 6.649 | -8.518 | 26.625 | 1.00 | 20.31 |
| | ATOM | 2618 | O | LEU | B | 391 | 7.002 | -9.352 | 27.465 | 1.00 | 18.66 |
| 15 | ATOM | 2619 | N | VAL | B | 392 | 7.378 | -8.215 | 25.557 | 1.00 | 18.71 |
| | ATOM | 2620 | CA | VAL | B | 392 | 8.649 | -8.868 | 25.278 | 1.00 | 19.51 |
| | ATOM | 2621 | CB | VAL | B | 392 | 9.288 | -8.281 | 24.005 | 1.00 | 23.77 |
| | ATOM | 2622 | CG1 | VAL | B | 392 | 10.751 | -8.687 | 23.920 | 1.00 | 24.63 |
| | ATOM | 2623 | CG2 | VAL | B | 392 | 8.520 | -8.773 | 22.767 | 1.00 | 19.94 |
| 20 | ATOM | 2624 | C | VAL | B | 392 | 9.615 | -8.707 | 26.450 | 1.00 | 22.80 |
| | ATOM | 2625 | O | VAL | B | 392 | 10.336 | -9.637 | 26.811 | 1.00 | 19.36 |
| | ATOM | 2626 | N | TRP | B | 393 | 9.617 | -7.522 | 27.046 | 1.00 | 22.10 |
| | ATOM | 2627 | CA | TRP | B | 393 | 10.492 | -7.241 | 28.171 | 1.00 | 23.20 |
| | ATOM | 2628 | CB | TRP | B | 393 | 10.388 | -5.773 | 28.578 | 1.00 | 19.22 |
| 25 | ATOM | 2629 | CG | TRP | B | 393 | 11.056 | -5.479 | 29.895 | 1.00 | 22.53 |
| | ATOM | 2630 | CD2 | TRP | B | 393 | 12.453 | -5.591 | 30.193 | 1.00 | 20.36 |
| | ATOM | 2631 | CE2 | TRP | B | 393 | 12.624 | -5.208 | 31.545 | 1.00 | 25.65 |
| | ATOM | 2632 | CE3 | TRP | B | 393 | 13.578 | -5.976 | 29.449 | 1.00 | 22.12 |
| | ATOM | 2633 | CD1 | TRP | B | 393 | 10.452 | -5.046 | 31.044 | 1.00 | 23.02 |
| 30 | ATOM | 2634 | NE1 | TRP | B | 393 | 11.387 | -4.881 | 32.037 | 1.00 | 24.91 |
| | ATOM | 2635 | CZ2 | TRP | B | 393 | 13.876 | -5.200 | 32.171 | 1.00 | 23.00 |
| | ATOM | 2636 | CZ3 | TRP | B | 393 | 14.829 | -5.968 | 30.072 | 1.00 | 23.98 |
| | ATOM | 2637 | CH2 | TRP | B | 393 | 14.964 | -5.582 | 31.423 | 1.00 | 23.20 |
| | ATOM | 2638 | C | TRP | B | 393 | 10.208 | -8.114 | 29.388 | 1.00 | 24.36 |
| 35 | ATOM | 2639 | O | TRP | B | 393 | 11.128 | -8.717 | 29.944 | 1.00 | 23.04 |
| | ATOM | 2640 | N | ARG | B | 394 | 8.952 | -8.189 | 29.819 | 1.00 | 21.29 |
| | ATOM | 2641 | CA | ARG | B | 394 | 8.680 | -9.003 | 30.990 | 1.00 | 22.43 |
| | ATOM | 2642 | CB | ARG | B | 394 | 7.365 | -8.601 | 31.667 | 1.00 | 23.97 |
| | ATOM | 2643 | CG | ARG | B | 394 | 6.259 | -8.149 | 30.759 | 1.00 | 26.16 |
| 40 | ATOM | 2644 | CD | ARG | B | 394 | 5.026 | -7.727 | 31.574 | 1.00 | 20.86 |
| | ATOM | 2645 | NE | ARG | B | 394 | 3.817 | -7.937 | 30.786 | 1.00 | 19.54 |
| | ATOM | 2646 | CZ | ARG | B | 394 | 3.327 | -7.059 | 29.915 | 1.00 | 20.58 |
| | ATOM | 2647 | NH1 | ARG | B | 394 | 3.944 | -5.902 | 29.722 | 1.00 | 17.41 |
| | ATOM | 2648 | NH2 | ARG | B | 394 | 2.229 | -7.347 | 29.220 | 1.00 | 16.82 |
| 45 | ATOM | 2649 | C | ARG | B | 394 | 8.695 | -10.502 | 30.713 | 1.00 | 21.78 |
| | ATOM | 2650 | O | ARG | B | 394 | 8.657 | -11.294 | 31.648 | 1.00 | 23.44 |
| | ATOM | 2651 | N | SER | B | 395 | 8.767 | -10.880 | 29.438 | 1.00 | 17.10 |
| | ATOM | 2652 | CA | SER | B | 395 | 8.805 | -12.289 | 29.041 | 1.00 | 25.08 |
| | ATOM | 2653 | CB | SER | B | 395 | 8.206 | -12.473 | 27.638 | 1.00 | 19.47 |
| 50 | ATOM | 2654 | OG | SER | B | 395 | 6.832 | -12.136 | 27.619 | 1.00 | 21.73 |
| | ATOM | 2655 | C | SER | B | 395 | 10.239 | -12.831 | 29.031 | 1.00 | 26.29 |
| | ATOM | 2656 | O | SER | B | 395 | 10.458 | -14.030 | 28.854 | 1.00 | 23.75 |
| | ATOM | 2657 | N | MET | B | 396 | 11.206 | -11.938 | 29.210 | 1.00 | 30.79 |
| | ATOM | 2658 | CA | MET | B | 396 | 12.620 | -12.307 | 29.205 | 1.00 | 35.07 |
| 55 | ATOM | 2659 | CB | MET | B | 396 | 13.479 | -11.063 | 29.423 | 1.00 | 33.84 |
| | ATOM | 2660 | CG | MET | B | 396 | 14.155 | -10.569 | 28.171 | 1.00 | 36.88 |
| | ATOM | 2661 | SD | MET | B | 396 | 15.149 | -9.127 | 28.491 | 1.00 | 40.96 |
| | ATOM | 2662 | CE | MET | B | 396 | 16.675 | -9.849 | 28.998 | 1.00 | 39.67 |
| | ATOM | 2663 | C | MET | B | 396 | 12.983 | -13.353 | 30.250 | 1.00 | 35.88 |
| 60 | ATOM | 2664 | O | MET | B | 396 | 13.828 | -14.215 | 30.011 | 1.00 | 34.52 |
| | ATOM | 2665 | N | GLU | B | 397 | 12.348 | -13.266 | 31.410 | 1.00 | 36.19 |

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|----|------|------|-----|-----|---|-----|--------|--------------------------|------|-------|
| 5 | ATOM | 2666 | CA | GLU | B | 397 | 12.604 | 11.208 32.492 | 1.00 | 39.24 |
| | ATOM | 2667 | CB | GLU | B | 397 | 12.153 | -13.605 33.821 | 1.00 | 44.38 |
| | ATOM | 2668 | CG | GLU | B | 397 | 12.983 | -12.422 34.271 | 1.00 | 54.05 |
| | ATOM | 2669 | CD | GLU | B | 397 | 13.483 | -12.587 35.686 | 1.00 | 56.78 |
| | ATOM | 2670 | OE1 | GLU | B | 397 | 13.380 | -11.621 36.470 | 1.00 | 60.90 |
| 10 | ATOM | 2671 | OE2 | GLU | B | 397 | 13.975 | -13.688 36.013 | 1.00 | 60.82 |
| | ATOM | 2672 | C | GLU | B | 397 | 11.878 | -15.528 32.273 | 1.00 | 36.65 |
| | ATOM | 2673 | O | GLU | B | 397 | 12.021 | -16.459 33.061 | 1.00 | 35.84 |
| | ATOM | 2674 | N | HIS | B | 398 | 11.100 | -15.609 31.202 | 1.00 | 32.14 |
| | ATOM | 2675 | CA | HIS | B | 398 | 10.347 | -16.823 30.914 | 1.00 | 29.48 |
| 15 | ATOM | 2676 | CB | HIS | B | 398 | 8.863 | -16.567 31.178 | 1.00 | 29.87 |
| | ATOM | 2677 | CG | HIS | B | 398 | 8.582 | -16.111 32.574 | 1.00 | 31.80 |
| | ATOM | 2678 | CD2 | HIS | B | 398 | 8.215 | -16.801 33.678 | 1.00 | 29.12 |
| | ATOM | 2679 | ND1 | HIS | B | 398 | 8.727 | -14.799 32.972 | 1.00 | 33.27 |
| | ATOM | 2680 | CE1 | HIS | B | 398 | 8.462 | -14.701 34.262 | 1.00 | 32.19 |
| 20 | ATOM | 2681 | NE2 | HIS | B | 398 | 8.148 | -15.902 34.714 | 1.00 | 33.48 |
| | ATOM | 2682 | C | HIS | B | 398 | 10.556 | -17.317 29.492 | 1.00 | 25.95 |
| | ATOM | 2683 | O | HIS | B | 398 | 9.637 | -17.291 28.672 | 1.00 | 27.47 |
| | ATOM | 2684 | N | PRO | B | 399 | 11.771 | -17.801 29.186 | 1.00 | 29.09 |
| | ATOM | 2685 | CD | PRO | B | 399 | 12.926 | -17.922 30.096 | 1.00 | 29.93 |
| 25 | ATOM | 2686 | CA | PRO | B | 399 | 12.079 | -18.300 27.845 | 1.00 | 27.40 |
| | ATOM | 2687 | CB | PRO | B | 399 | 13.434 | -18.988 28.016 | 1.00 | 32.09 |
| | ATOM | 2688 | CG | PRO | B | 399 | 14.062 | -18.284 29.170 | 1.00 | 30.81 |
| | ATOM | 2689 | C | PRO | B | 399 | 11.009 | -19.246 27.319 | 1.00 | 29.76 |
| | ATOM | 2690 | O | PRO | B | 399 | 10.552 | -20.137 28.035 | 1.00 | 29.18 |
| 30 | ATOM | 2691 | N | GLY | B | 400 | 10.601 | -19.035 26.071 | 1.00 | 27.45 |
| | ATOM | 2692 | CA | GLY | B | 400 | 9.588 | -19.884 25.466 | 1.00 | 26.93 |
| | ATOM | 2693 | C | GLY | B | 400 | 8.161 | -19.537 25.849 | 1.00 | 26.73 |
| | ATOM | 2694 | O | GLY | B | 400 | 7.220 | -20.153 25.356 | 1.00 | 28.36 |
| | ATOM | 2695 | N | LYS | B | 401 | 7.996 | -18.554 26.727 | 1.00 | 25.50 |
| 35 | ATOM | 2696 | CA | LYS | B | 401 | 6.668 | -18.139 27.165 | 1.00 | 23.45 |
| | ATOM | 2697 | CB | LYS | B | 401 | 6.435 | -18.563 28.619 | 1.00 | 28.50 |
| | ATOM | 2698 | CG | LYS | B | 401 | 6.476 | -20.069 28.879 | 1.00 | 28.58 |
| | ATOM | 2699 | CD | LYS | B | 401 | 6.181 | -20.353 30.349 | 1.00 | 35.47 |
| | ATOM | 2700 | CE | LYS | B | 401 | 6.073 | -21.847 30.635 | 1.00 | 38.59 |
| 40 | ATOM | 2701 | NZ | LYS | B | 401 | 7.177 | -22.611 29.989 | 1.00 | 42.39 |
| | ATOM | 2702 | C | LYS | B | 401 | 6.493 | -16.622 27.060 | 1.00 | 21.78 |
| | ATOM | 2703 | O | LYS | B | 401 | 7.465 | -15.872 27.035 | 1.00 | 21.45 |
| | ATOM | 2704 | N | LEU | B | 402 | 5.241 | -16.181 26.995 | 1.00 | 23.45 |
| | ATOM | 2705 | CA | LEU | B | 402 | 4.929 | -14.759 26.925 | 1.00 | 21.37 |
| 45 | ATOM | 2706 | CB | LEU | B | 402 | 4.088 | -14.449 25.689 | 1.00 | 18.47 |
| | ATOM | 2707 | CG | LEU | B | 402 | 4.798 | -14.673 24.360 | 1.00 | 16.89 |
| | ATOM | 2708 | CD1 | LEU | B | 402 | 3.821 | -14.395 23.211 | 1.00 | 21.23 |
| | ATOM | 2709 | CD2 | LEU | B | 402 | 6.011 | -13.760 24.277 | 1.00 | 23.15 |
| | ATOM | 2710 | C | LEU | B | 402 | 4.147 | -14.399 28.179 | 1.00 | 19.66 |
| 50 | ATOM | 2711 | O | LEU | B | 402 | 3.024 | -14.880 28.381 | 1.00 | 18.05 |
| | ATOM | 2712 | N | LEU | B | 403 | 4.743 | -13.559 29.019 | 1.00 | 19.54 |
| | ATOM | 2713 | CA | LEU | B | 403 | 4.099 | -13.148 30.259 | 1.00 | 20.21 |
| | ATOM | 2714 | CB | LEU | B | 403 | 5.155 | -12.856 31.332 | 1.00 | 23.16 |
| | ATOM | 2715 | CG | LEU | B | 403 | 4.639 | -12.682 32.766 | 1.00 | 29.54 |
| 55 | ATOM | 2716 | CD1 | LEU | B | 403 | 5.519 | -13.450 33.728 | 1.00 | 32.67 |
| | ATOM | 2717 | CD2 | LEU | B | 403 | 4.626 | -11.213 33.138 | 1.00 | 32.38 |
| | ATOM | 2718 | C | LEU | B | 403 | 3.219 | -11.918 30.043 | 1.00 | 20.42 |
| | ATOM | 2719 | O | LEU | B | 403 | 3.638 | -10.787 30.291 | 1.00 | 19.18 |
| | ATOM | 2720 | N | PHE | B | 404 | 2.003 | -12.145 29.565 | 1.00 | 21.44 |
| 60 | ATOM | 2721 | CA | PHE | B | 404 | 1.066 | -11.053 29.340 | 1.00 | 21.69 |
| | ATOM | 2722 | CB | PHE | B | 404 | -0.199 | -11.598 28.687 | 1.00 | 17.26 |

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 2723 | CG | PHE | B | 404 | -0.026 | -11.897 | 27.227 | 1.00 | 19.75 |
| | ATOM | 2724 | CD1 | PHE | B | 404 | 0.364 | -13.167 | 26.801 | 1.00 | 17.90 |
| | ATOM | 2725 | CD2 | PHE | B | 404 | -0.210 | -10.897 | 26.280 | 1.00 | 17.04 |
| | ATOM | 2726 | CE1 | PHE | B | 404 | 0.572 | -13.434 | 25.447 | 1.00 | 19.88 |
| | ATOM | 2727 | CE2 | PHE | B | 404 | -0.007 | -11.148 | 24.924 | 1.00 | 18.47 |
| 10 | ATOM | 2728 | CZ | PHE | B | 404 | 0.386 | -12.418 | 24.503 | 1.00 | 16.45 |
| | ATOM | 2729 | C | PHE | B | 404 | 0.768 | -10.403 | 30.685 | 1.00 | 21.95 |
| | ATOM | 2730 | O | PHE | B | 404 | 0.656 | -9.177 | 30.804 | 1.00 | 22.99 |
| | ATOM | 2731 | N | ALA | B | 405 | 0.670 | -11.247 | 31.702 | 1.00 | 21.12 |
| | ATOM | 2732 | CA | ALA | B | 405 | 0.424 | -10.814 | 33.066 | 1.00 | 22.43 |
| 15 | ATOM | 2733 | CB | ALA | B | 405 | -1.074 | -10.603 | 33.304 | 1.00 | 24.69 |
| | ATOM | 2734 | C | ALA | B | 405 | 0.959 | -11.926 | 33.962 | 1.00 | 22.40 |
| | ATOM | 2735 | O | ALA | B | 405 | 1.133 | -13.061 | 33.517 | 1.00 | 21.67 |
| | ATOM | 2736 | N | PRO | B | 406 | 1.246 | -11.612 | 35.230 | 1.00 | 25.60 |
| | ATOM | 2737 | CD | PRO | B | 406 | 1.129 | -10.294 | 35.878 | 1.00 | 23.65 |
| 20 | ATOM | 2738 | CA | PRO | B | 406 | 1.765 | -12.632 | 36.148 | 1.00 | 25.91 |
| | ATOM | 2739 | CB | PRO | B | 406 | 1.899 | -11.882 | 37.475 | 1.00 | 27.04 |
| | ATOM | 2740 | CG | PRO | B | 406 | 2.017 | -10.431 | 37.068 | 1.00 | 26.56 |
| | ATOM | 2741 | C | PRO | B | 406 | 0.876 | -13.873 | 36.259 | 1.00 | 25.12 |
| | ATOM | 2742 | O | PRO | B | 406 | 1.368 | -14.967 | 36.538 | 1.00 | 28.92 |
| 25 | ATOM | 2743 | N | ASN | B | 407 | -0.426 | -13.713 | 36.039 | 1.00 | 23.53 |
| | ATOM | 2744 | CA | ASN | B | 407 | -1.345 | -14.852 | 36.109 | 1.00 | 24.09 |
| | ATOM | 2745 | CB | ASN | B | 407 | -2.553 | -14.526 | 36.986 | 1.00 | 24.08 |
| | ATOM | 2746 | CG | ASN | B | 407 | -3.327 | -13.328 | 36.486 | 1.00 | 26.72 |
| | ATOM | 2747 | OD1 | ASN | B | 407 | -2.851 | -12.574 | 35.635 | 1.00 | 22.65 |
| 30 | ATOM | 2748 | ND2 | ASN | B | 407 | -4.528 | -13.140 | 37.019 | 1.00 | 26.46 |
| | ATOM | 2749 | C | ASN | B | 407 | -1.820 | -15.231 | 34.714 | 1.00 | 26.91 |
| | ATOM | 2750 | O | ASN | B | 407 | -2.859 | -15.870 | 34.548 | 1.00 | 28.68 |
| | ATOM | 2751 | N | LEU | B | 408 | -1.059 | -14.816 | 33.708 | 1.00 | 27.28 |
| | ATOM | 2752 | CA | LEU | B | 408 | -1.387 | -15.124 | 32.327 | 1.00 | 27.23 |
| 35 | ATOM | 2753 | CB | LEU | B | 408 | -2.247 | -14.030 | 31.699 | 1.00 | 26.61 |
| | ATOM | 2754 | CG | LEU | B | 408 | -2.815 | -14.464 | 30.341 | 1.00 | 27.51 |
| | ATOM | 2755 | CD1 | LEU | B | 408 | -3.702 | -15.692 | 30.546 | 1.00 | 28.75 |
| | ATOM | 2756 | CD2 | LEU | B | 408 | -3.598 | -13.330 | 29.694 | 1.00 | 25.48 |
| | ATOM | 2757 | C | LEU | B | 408 | -0.113 | -15.316 | 31.514 | 1.00 | 27.56 |
| 40 | ATOM | 2758 | O | LEU | B | 408 | 0.247 | -14.465 | 30.695 | 1.00 | 26.86 |
| | ATOM | 2759 | N | LEU | B | 409 | 0.553 | -16.426 | 31.759 | 1.00 | 27.54 |
| | ATOM | 2760 | CA | LEU | B | 409 | 1.786 | -16.774 | 31.065 | 1.00 | 31.96 |
| | ATOM | 2761 | CB | LEU | B | 409 | 2.786 | -17.355 | 32.058 | 1.00 | 31.88 |
| | ATOM | 2762 | CG | LEU | B | 409 | 4.186 | -17.703 | 31.562 | 1.00 | 37.72 |
| 45 | ATOM | 2763 | CD1 | LEU | B | 409 | 4.773 | -16.551 | 30.770 | 1.00 | 39.57 |
| | ATOM | 2764 | CD2 | LEU | B | 409 | 5.066 | -18.018 | 32.758 | 1.00 | 41.72 |
| | ATOM | 2765 | C | LEU | B | 409 | 1.401 | -17.805 | 30.009 | 1.00 | 31.53 |
| | ATOM | 2766 | O | LEU | B | 409 | 0.921 | -18.892 | 30.340 | 1.00 | 32.67 |
| | ATOM | 2767 | N | LEU | B | 410 | 1.604 | -17.465 | 28.746 | 1.00 | 29.58 |
| 50 | ATOM | 2768 | CA | LEU | B | 410 | 1.228 | -18.361 | 27.660 | 1.00 | 31.55 |
| | ATOM | 2769 | CB | LEU | B | 410 | 0.192 | -17.672 | 26.762 | 1.00 | 29.83 |
| | ATOM | 2770 | CG | LEU | B | 410 | -1.047 | -17.080 | 27.452 | 1.00 | 28.55 |
| | ATOM | 2771 | CD1 | LEU | B | 410 | -1.770 | -16.135 | 26.501 | 1.00 | 26.92 |
| | ATOM | 2772 | CD2 | LEU | B | 410 | -1.979 | -18.200 | 27.891 | 1.00 | 30.49 |
| 55 | ATOM | 2773 | C | LEU | B | 410 | 2.397 | -18.839 | 26.814 | 1.00 | 33.88 |
| | ATOM | 2774 | O | LEU | B | 410 | 3.427 | -18.170 | 26.726 | 1.00 | 36.49 |
| | ATOM | 2775 | N | ASP | B | 411 | 2.238 | -20.013 | 26.206 | 1.00 | 38.80 |
| | ATOM | 2776 | CA | ASP | B | 411 | 3.275 | -20.562 | 25.336 | 1.00 | 38.39 |
| | ATOM | 2777 | CB | ASP | B | 411 | 3.657 | -21.990 | 25.752 | 1.00 | 44.53 |
| 60 | ATOM | 2778 | CG | ASP | B | 411 | 2.476 | -22.943 | 25.749 | 1.00 | 44.90 |
| | ATOM | 2779 | OD1 | ASP | B | 411 | 1.773 | -23.035 | 24.719 | 1.00 | 45.70 |

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 2780 | OD2 | ASP | B | 411 | 2.254 | -23.603 | 26.786 | 1.00 | 50.54 |
| | ATOM | 2781 | C | ASP | B | 411 | 2.745 | -20.551 | 23.909 | 1.00 | 38.57 |
| | ATOM | 2782 | O | ASP | B | 411 | 1.549 | -20.341 | 23.686 | 1.00 | 36.48 |
| | ATOM | 2783 | N | ARG | B | 412 | 3.635 | -20.777 | 22.949 | 1.00 | 36.85 |
| | ATOM | 2784 | CA | ARG | B | 412 | 3.259 | -20.763 | 21.541 | 1.00 | 38.32 |
| 10 | ATOM | 2785 | CB | ARG | B | 412 | 4.488 | -21.083 | 20.675 | 1.00 | 38.69 |
| | ATOM | 2786 | CG | ARG | B | 412 | 4.361 | -22.314 | 19.799 | 1.00 | 40.05 |
| | ATOM | 2787 | CD | ARG | B | 412 | 5.644 | -22.552 | 19.012 | 1.00 | 42.98 |
| | ATOM | 2788 | NE | ARG | B | 412 | 5.540 | -22.099 | 17.626 | 1.00 | 40.95 |
| | ATOM | 2789 | CZ | ARG | B | 412 | 4.649 | -22.559 | 16.753 | 1.00 | 41.11 |
| 15 | ATOM | 2790 | NH1 | ARG | B | 412 | 3.777 | -23.490 | 17.115 | 1.00 | 44.01 |
| | ATOM | 2791 | NH2 | ARG | B | 412 | 4.632 | -22.091 | 15.515 | 1.00 | 41.28 |
| | ATOM | 2792 | C | ARG | B | 412 | 2.107 | -21.712 | 21.217 | 1.00 | 37.64 |
| | ATOM | 2793 | O | ARG | B | 412 | 1.287 | -21.427 | 20.343 | 1.00 | 36.51 |
| | ATOM | 2794 | N | ASN | B | 413 | 2.041 | -22.834 | 21.923 | 1.00 | 35.32 |
| 20 | ATOM | 2795 | CA | ASN | B | 413 | 0.974 | -23.798 | 21.688 | 1.00 | 36.68 |
| | ATOM | 2796 | CB | ASN | B | 413 | 1.170 | -25.035 | 22.570 | 1.00 | 37.54 |
| | ATOM | 2797 | CG | ASN | B | 413 | 2.017 | -26.100 | 21.901 | 1.00 | 43.56 |
| | ATOM | 2798 | OD1 | ASN | B | 413 | 2.309 | -26.022 | 20.704 | 1.00 | 46.11 |
| | ATOM | 2799 | ND2 | ASN | B | 413 | 2.418 | -27.104 | 22.671 | 1.00 | 47.04 |
| 25 | ATOM | 2800 | C | ASN | B | 413 | -0.383 | -23.168 | 21.982 | 1.00 | 34.01 |
| | ATOM | 2801 | O | ASN | B | 413 | -1.349 | -23.372 | 21.247 | 1.00 | 32.43 |
| | ATOM | 2802 | N | GLN | B | 414 | -0.447 | -22.397 | 23.063 | 1.00 | 32.85 |
| | ATOM | 2803 | CA | GLN | B | 414 | -1.685 | -21.741 | 23.449 | 1.00 | 31.91 |
| | ATOM | 2804 | CB | GLN | B | 414 | -1.558 | -21.172 | 24.863 | 1.00 | 33.17 |
| 30 | ATOM | 2805 | CG | GLN | B | 414 | -1.528 | -22.242 | 25.948 | 1.00 | 32.31 |
| | ATOM | 2806 | CD | GLN | B | 414 | -1.293 | -21.667 | 27.327 | 1.00 | 34.63 |
| | ATOM | 2807 | OE1 | GLN | B | 414 | -0.176 | -21.277 | 27.666 | 1.00 | 33.23 |
| | ATOM | 2808 | NE2 | GLN | B | 414 | -2.349 | -21.606 | 28.131 | 1.00 | 34.56 |
| | ATOM | 2809 | C | GLN | B | 414 | -2.052 | -20.638 | 22.463 | 1.00 | 29.57 |
| 35 | ATOM | 2810 | O | GLN | B | 414 | -3.195 | -20.204 | 22.409 | 1.00 | 31.32 |
| | ATOM | 2811 | N | GLY | B | 415 | -1.077 | -20.190 | 21.682 | 1.00 | 30.96 |
| | ATOM | 2812 | CA | GLY | B | 415 | -1.350 | -19.160 | 20.697 | 1.00 | 34.27 |
| | ATOM | 2813 | C | GLY | B | 415 | -2.184 | -19.725 | 19.562 | 1.00 | 35.27 |
| | ATOM | 2814 | O | GLY | B | 415 | -2.918 | -19.000 | 18.887 | 1.00 | 33.20 |
| 40 | ATOM | 2815 | N | LYS | B | 416 | -2.070 | -21.031 | 19.354 | 1.00 | 35.28 |
| | ATOM | 2816 | CA | LYS | B | 416 | -2.819 | -21.707 | 18.299 | 1.00 | 38.26 |
| | ATOM | 2817 | CB | LYS | B | 416 | -2.398 | -23.177 | 18.201 | 1.00 | 38.00 |
| | ATOM | 2818 | CG | LYS | B | 416 | -0.973 | -23.407 | 17.736 | 1.00 | 40.05 |
| | ATOM | 2819 | CD | LYS | B | 416 | -0.405 | -24.668 | 18.369 | 1.00 | 44.10 |
| 45 | ATOM | 2820 | CE | LYS | B | 416 | 0.306 | -25.541 | 17.346 | 1.00 | 41.85 |
| | ATOM | 2821 | NZ | LYS | B | 416 | 1.286 | -24.760 | 16.542 | 1.00 | 45.63 |
| | ATOM | 2822 | C | LYS | B | 416 | -4.321 | -21.645 | 18.559 | 1.00 | 36.93 |
| | ATOM | 2823 | O | LYS | B | 416 | -5.121 | -21.790 | 17.638 | 1.00 | 38.36 |
| | ATOM | 2824 | N | CYS | B | 417 | -4.698 | -21.430 | 19.817 | 1.00 | 37.10 |
| 50 | ATOM | 2825 | CA | CYS | B | 417 | -6.106 | -21.371 | 20.196 | 1.00 | 36.46 |
| | ATOM | 2826 | CB | CYS | B | 417 | -6.218 | -21.226 | 21.717 | 1.00 | 39.01 |
| | ATOM | 2827 | SG | CYS | B | 417 | -5.674 | -22.710 | 22.612 | 1.00 | 43.81 |
| | ATOM | 2828 | C | CYS | B | 417 | -6.899 | -20.277 | 19.491 | 1.00 | 35.19 |
| | ATOM | 2829 | O | CYS | B | 417 | -8.127 | -20.296 | 19.485 | 1.00 | 33.92 |
| 55 | ATOM | 2830 | N | VAL | B | 418 | -6.195 | -19.316 | 18.906 | 1.00 | 36.04 |
| | ATOM | 2831 | CA | VAL | B | 418 | -6.838 | -18.236 | 18.163 | 1.00 | 34.59 |
| | ATOM | 2832 | CB | VAL | B | 418 | -6.525 | -16.850 | 18.775 | 1.00 | 34.87 |
| | ATOM | 2833 | CG1 | VAL | B | 418 | -6.831 | -15.763 | 17.765 | 1.00 | 35.32 |
| | ATOM | 2834 | CG2 | VAL | B | 418 | -7.350 | -16.630 | 20.036 | 1.00 | 33.65 |
| 60 | ATOM | 2835 | C | VAL | B | 418 | -6.241 | -18.317 | 16.764 | 1.00 | 34.17 |
| | ATOM | 2836 | O | VAL | B | 418 | -5.020 | -18.323 | 16.611 | 1.00 | 32.73 |

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|----|------|------|-----|-----|---|-----|---------|---------|--------|------|-------|
| 5 | ATOM | 2837 | N | GLU | B | 419 | -7.084 | -18.388 | 15.740 | 1.00 | 33.44 |
| | ATOM | 2838 | CA | GLU | B | 419 | -6.554 | -18.500 | 14.390 | 1.00 | 34.52 |
| | ATOM | 2839 | CB | GLU | B | 419 | -7.681 | -18.722 | 13.380 | 1.00 | 36.21 |
| | ATOM | 2840 | CG | GLU | B | 419 | -8.597 | -17.538 | 13.166 | 1.00 | 44.19 |
| | ATOM | 2841 | CD | GLU | B | 419 | -9.477 | -17.723 | 11.946 | 1.00 | 48.47 |
| 10 | ATOM | 2842 | OE1 | GLU | B | 419 | -9.157 | -18.605 | 11.119 | 1.00 | 51.04 |
| | ATOM | 2843 | OE2 | GLU | B | 419 | -10.484 | -16.993 | 11.813 | 1.00 | 48.91 |
| | ATOM | 2844 | C | GLU | B | 419 | -5.717 | -17.289 | 13.997 | 1.00 | 32.89 |
| | ATOM | 2845 | O | GLU | B | 419 | -6.156 | -16.144 | 14.123 | 1.00 | 31.09 |
| | ATOM | 2846 | N | GLY | B | 420 | -4.501 | -17.562 | 13.535 | 1.00 | 32.84 |
| 15 | ATOM | 2847 | CA | GLY | B | 420 | -3.594 | -16.506 | 13.122 | 1.00 | 34.37 |
| | ATOM | 2848 | C | GLY | B | 420 | -2.722 | -15.955 | 14.240 | 1.00 | 35.30 |
| | ATOM | 2849 | O | GLY | B | 420 | -1.745 | -15.246 | 13.975 | 1.00 | 35.94 |
| | ATOM | 2850 | N | MET | B | 421 | -3.052 | -16.285 | 15.486 | 1.00 | 30.08 |
| | ATOM | 2851 | CA | MET | B | 421 | -2.289 | -15.780 | 16.625 | 1.00 | 29.22 |
| 20 | ATOM | 2852 | CB | MET | B | 421 | -3.108 | -15.922 | 17.914 | 1.00 | 22.54 |
| | ATOM | 2853 | CG | MET | B | 421 | -2.469 | -15.270 | 19.124 | 1.00 | 23.82 |
| | ATOM | 2854 | SD | MET | B | 421 | -2.124 | -13.494 | 18.872 | 1.00 | 28.40 |
| | ATOM | 2855 | CE | MET | B | 421 | -3.697 | -12.800 | 19.233 | 1.00 | 24.67 |
| | ATOM | 2856 | C | MET | B | 421 | -0.912 | -16.416 | 16.821 | 1.00 | 29.67 |
| 25 | ATOM | 2857 | O | MET | B | 421 | 0.022 | -15.751 | 17.269 | 1.00 | 29.76 |
| | ATOM | 2858 | N | VAL | B | 422 | -0.766 | -17.694 | 16.484 | 1.00 | 30.63 |
| | ATOM | 2859 | CA | VAL | B | 422 | 0.524 | -18.338 | 16.675 | 1.00 | 29.90 |
| | ATOM | 2860 | CB | VAL | B | 422 | 0.482 | -19.835 | 16.273 | 1.00 | 35.74 |
| | ATOM | 2861 | CG1 | VAL | B | 422 | 0.514 | -19.992 | 14.753 | 1.00 | 37.64 |
| 30 | ATOM | 2862 | CG2 | VAL | B | 422 | 1.659 | -20.555 | 16.897 | 1.00 | 31.68 |
| | ATOM | 2863 | C | VAL | B | 422 | 1.669 | -17.640 | 15.935 | 1.00 | 28.64 |
| | ATOM | 2864 | O | VAL | B | 422 | 2.788 | -17.571 | 16.441 | 1.00 | 26.15 |
| | ATOM | 2865 | N | GLU | B | 423 | 1.402 | -17.113 | 14.747 | 1.00 | 28.70 |
| | ATOM | 2866 | CA | GLU | B | 423 | 2.454 | -16.435 | 13.997 | 1.00 | 31.34 |
| 35 | ATOM | 2867 | CB | GLU | B | 423 | 1.963 | -16.050 | 12.596 | 1.00 | 36.21 |
| | ATOM | 2868 | CG | GLU | B | 423 | 0.502 | -16.376 | 12.325 | 1.00 | 45.83 |
| | ATOM | 2869 | CD | GLU | B | 423 | 0.250 | -17.865 | 12.144 | 1.00 | 46.71 |
| | ATOM | 2870 | OE1 | GLU | B | 423 | -0.746 | -18.368 | 12.706 | 1.00 | 45.97 |
| | ATOM | 2871 | OE2 | GLU | B | 423 | 1.045 | -18.530 | 11.442 | 1.00 | 50.05 |
| 40 | ATOM | 2872 | C | GLU | B | 423 | 2.928 | -15.186 | 14.744 | 1.00 | 30.57 |
| | ATOM | 2873 | O | GLU | B | 423 | 4.119 | -14.870 | 14.759 | 1.00 | 26.59 |
| | ATOM | 2874 | N | ILE | B | 424 | 2.001 | -14.478 | 15.378 | 1.00 | 26.19 |
| | ATOM | 2875 | CA | ILE | B | 424 | 2.381 | -13.279 | 16.111 | 1.00 | 26.23 |
| | ATOM | 2876 | CB | ILE | B | 424 | 1.134 | -12.435 | 16.452 | 1.00 | 29.33 |
| 45 | ATOM | 2877 | CG2 | ILE | B | 424 | 1.492 | -11.315 | 17.425 | 1.00 | 30.91 |
| | ATOM | 2878 | CG1 | ILE | B | 424 | 0.584 | -11.817 | 15.160 | 1.00 | 29.09 |
| | ATOM | 2879 | CD1 | ILE | B | 424 | -0.895 | -11.514 | 15.187 | 1.00 | 30.51 |
| | ATOM | 2880 | C | ILE | B | 424 | 3.153 | -13.673 | 17.370 | 1.00 | 24.22 |
| | ATOM | 2881 | O | ILE | B | 424 | 4.152 | -13.037 | 17.725 | 1.00 | 21.05 |
| 50 | ATOM | 2882 | N | PHE | B | 425 | 2.708 | -14.746 | 18.023 | 1.00 | 21.71 |
| | ATOM | 2883 | CA | PHE | B | 425 | 3.370 | -15.236 | 19.223 | 1.00 | 18.85 |
| | ATOM | 2884 | CB | PHE | B | 425 | 2.650 | -16.479 | 19.768 | 1.00 | 22.98 |
| | ATOM | 2885 | CG | PHE | B | 425 | 1.580 | -16.183 | 20.795 | 1.00 | 22.17 |
| | ATOM | 2886 | CD1 | PHE | B | 425 | 1.287 | -17.112 | 21.792 | 1.00 | 25.47 |
| 55 | ATOM | 2887 | CD2 | PHE | B | 425 | 0.843 | -15.001 | 20.747 | 1.00 | 26.30 |
| | ATOM | 2888 | CE1 | PHE | B | 425 | 0.273 | -16.871 | 22.724 | 1.00 | 24.33 |
| | ATOM | 2889 | CE2 | PHE | B | 425 | -0.174 | -14.749 | 21.676 | 1.00 | 25.03 |
| | ATOM | 2890 | CZ | PHE | B | 425 | -0.459 | -15.684 | 22.663 | 1.00 | 26.44 |
| | ATOM | 2891 | C | PHE | B | 425 | 4.817 | -15.610 | 18.885 | 1.00 | 20.00 |
| 60 | ATOM | 2892 | O | PHE | B | 425 | 5.741 | -15.292 | 19.636 | 1.00 | 21.15 |
| | ATOM | 2893 | N | ASP | B | 426 | 5.023 | -16.281 | 17.754 | 1.00 | 19.87 |

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 2894 | CA | ASP | B | 426 | 6.378 | -16.685 | 17.377 | 1.00 | 23.20 |
| | ATOM | 2895 | CB | ASP | B | 426 | 6.364 | -17.510 | 16.090 | 1.00 | 26.53 |
| | ATOM | 2896 | CG | ASP | B | 426 | 5.992 | -18.965 | 16.335 | 1.00 | 34.28 |
| | ATOM | 2897 | OD1 | ASP | B | 426 | 6.242 | -19.467 | 17.455 | 1.00 | 35.24 |
| | ATOM | 2898 | OD2 | ASP | B | 426 | 5.448 | -19.600 | 15.409 | 1.00 | 31.49 |
| 10 | ATOM | 2899 | C | ASP | B | 426 | 7.302 | -15.489 | 17.198 | 1.00 | 21.84 |
| | ATOM | 2900 | O | ASP | B | 426 | 8.465 | -15.526 | 17.593 | 1.00 | 21.55 |
| | ATOM | 2901 | N | MET | B | 427 | 6.788 | -14.429 | 16.591 | 1.00 | 20.12 |
| | ATOM | 2902 | CA | MET | B | 427 | 7.597 | -13.234 | 16.382 | 1.00 | 21.02 |
| | ATOM | 2903 | CB | MET | B | 427 | 6.836 | -12.228 | 15.520 | 1.00 | 18.53 |
| 15 | ATOM | 2904 | CG | MET | B | 427 | 6.864 | -12.559 | 14.038 | 1.00 | 27.92 |
| | ATOM | 2905 | SD | MET | B | 427 | 6.011 | -11.341 | 13.024 | 1.00 | 32.84 |
| | ATOM | 2906 | CE | MET | B | 427 | 4.363 | -11.532 | 13.581 | 1.00 | 33.63 |
| | ATOM | 2907 | C | MET | B | 427 | 7.945 | -12.616 | 17.732 | 1.00 | 17.42 |
| | ATOM | 2908 | O | MET | B | 427 | 9.073 | -12.180 | 17.950 | 1.00 | 22.09 |
| 20 | ATOM | 2909 | N | LEU | B | 428 | 6.968 | -12.597 | 18.634 | 1.00 | 20.47 |
| | ATOM | 2910 | CA | LEU | B | 428 | 7.157 | -12.033 | 19.968 | 1.00 | 20.13 |
| | ATOM | 2911 | CB | LEU | B | 428 | 5.812 | -11.964 | 20.706 | 1.00 | 17.58 |
| | ATOM | 2912 | CG | LEU | B | 428 | 4.852 | -10.887 | 20.179 | 1.00 | 18.41 |
| | ATOM | 2913 | CD1 | LEU | B | 428 | 3.443 | -11.155 | 20.687 | 1.00 | 11.95 |
| 25 | ATOM | 2914 | CD2 | LEU | B | 428 | 5.324 | -9.505 | 20.631 | 1.00 | 17.80 |
| | ATOM | 2915 | C | LEU | B | 428 | 8.159 | -12.856 | 20.767 | 1.00 | 20.68 |
| | ATOM | 2916 | O | LEU | B | 428 | 9.028 | -12.305 | 21.445 | 1.00 | 20.45 |
| | ATOM | 2917 | N | LEU | B | 429 | 8.037 | -14.178 | 20.679 | 1.00 | 20.35 |
| | ATOM | 2918 | CA | LEU | B | 429 | 8.938 | -15.082 | 21.382 | 1.00 | 19.82 |
| 30 | ATOM | 2919 | CB | LEU | B | 429 | 8.470 | -16.532 | 21.211 | 1.00 | 23.13 |
| | ATOM | 2920 | CG | LEU | B | 429 | 7.189 | -16.839 | 21.997 | 1.00 | 21.85 |
| | ATOM | 2921 | CD1 | LEU | B | 429 | 6.551 | -18.123 | 21.494 | 1.00 | 25.39 |
| | ATOM | 2922 | CD2 | LEU | B | 429 | 7.537 | -16.944 | 23.475 | 1.00 | 24.91 |
| | ATOM | 2923 | C | LEU | B | 429 | 10.361 | -14.936 | 20.865 | 1.00 | 20.74 |
| 35 | ATOM | 2924 | O | LEU | B | 429 | 11.318 | -14.968 | 21.638 | 1.00 | 21.02 |
| | ATOM | 2925 | N | ALA | B | 430 | 10.495 | -14.770 | 19.554 | 1.00 | 21.40 |
| | ATOM | 2926 | CA | ALA | B | 430 | 11.808 | -14.609 | 18.947 | 1.00 | 22.77 |
| | ATOM | 2927 | CB | ALA | B | 430 | 11.677 | -14.596 | 17.432 | 1.00 | 21.11 |
| | ATOM | 2928 | C | ALA | B | 430 | 12.467 | -13.315 | 19.440 | 1.00 | 22.40 |
| 40 | ATOM | 2929 | O | ALA | B | 430 | 13.670 | -13.277 | 19.713 | 1.00 | 20.62 |
| | ATOM | 2930 | N | THR | B | 431 | 11.670 | -12.258 | 19.567 | 1.00 | 21.09 |
| | ATOM | 2931 | CA | THR | B | 431 | 12.183 | -10.974 | 20.021 | 1.00 | 22.67 |
| | ATOM | 2932 | CB | THR | B | 431 | 11.128 | -9.866 | 19.863 | 1.00 | 23.77 |
| | ATOM | 2933 | OG1 | THR | B | 431 | 10.572 | -9.936 | 18.547 | 1.00 | 23.84 |
| 45 | ATOM | 2934 | CG2 | THR | B | 431 | 11.762 | -8.489 | 20.073 | 1.00 | 21.78 |
| | ATOM | 2935 | C | THR | B | 431 | 12.603 | -11.037 | 21.480 | 1.00 | 21.98 |
| | ATOM | 2936 | O | THR | B | 431 | 13.595 | -10.429 | 21.879 | 1.00 | 19.85 |
| | ATOM | 2937 | N | SER | B | 432 | 11.844 | -11.773 | 22.280 | 1.00 | 24.24 |
| | ATOM | 2938 | CA | SER | B | 432 | 12.169 | -11.906 | 23.693 | 1.00 | 26.96 |
| 50 | ATOM | 2939 | CB | SER | B | 432 | 11.055 | -12.661 | 24.423 | 1.00 | 28.00 |
| | ATOM | 2940 | OG | SER | B | 432 | 11.404 | -12.888 | 25.776 | 1.00 | 30.31 |
| | ATOM | 2941 | C | SER | B | 432 | 13.491 | -12.660 | 23.820 | 1.00 | 27.67 |
| | ATOM | 2942 | O | SER | B | 432 | 14.305 | -12.377 | 24.701 | 1.00 | 23.78 |
| | ATOM | 2943 | N | SER | B | 433 | 13.691 | -13.628 | 22.932 | 1.00 | 29.27 |
| 55 | ATOM | 2944 | CA | SER | B | 433 | 14.914 | -14.421 | 22.928 | 1.00 | 31.96 |
| | ATOM | 2945 | CB | SER | B | 433 | 14.790 | -15.575 | 21.938 | 1.00 | 30.84 |
| | ATOM | 2946 | OG | SER | B | 433 | 14.761 | -16.808 | 22.625 | 1.00 | 38.26 |
| | ATOM | 2947 | C | SER | B | 433 | 16.104 | -13.550 | 22.548 | 1.00 | 31.47 |
| | ATOM | 2948 | O | SER | B | 433 | 17.204 | -13.701 | 23.087 | 1.00 | 28.43 |
| 60 | ATOM | 2949 | N | ARG | B | 434 | 15.878 | -12.641 | 21.607 | 1.00 | 29.55 |
| | ATOM | 2950 | CA | ARG | B | 434 | 16.926 | -11.739 | 21.165 | 1.00 | 29.40 |

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|----|------|------|-----|------|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 2951 | CB | ARG | B | 434 | 16.437 | -10.912 | 19.977 | 1.00 | 31.56 |
| | ATOM | 2952 | CG | ARG | B | 434 | 17.428 | -9.868 | 19.493 | 1.00 | 36.76 |
| | ATOM | 2953 | CD | ARG | B | 434 | 18.694 | -10.502 | 18.919 | 1.00 | 37.76 |
| | ATOM | 2954 | NE | ARG | B | 434 | 19.654 | -9.479 | 18.516 | 1.00 | 39.50 |
| | ATOM | 2955 | CZ | ARG | B | 434 | 20.965 | -9.673 | 18.418 | 1.00 | 44.17 |
| 10 | ATOM | 2956 | NH1 | ARG | B | 434 | 21.492 | -10.861 | 18.696 | 1.00 | 43.17 |
| | ATOM | 2957 | NH2 | ARG | B | 434 | 21.750 | -8.671 | 18.048 | 1.00 | 43.05 |
| | ATOM | 2958 | C | ARG | B | 434 | 17.328 | -10.827 | 22.326 | 1.00 | 29.15 |
| | ATOM | 2959 | O | ARG | B | 434 | 18.515 | -10.612 | 22.569 | 1.00 | 28.82 |
| | ATOM | 2960 | N | PHE | B | 435 | 16.337 | -10.297 | 23.039 | 1.00 | 24.88 |
| 15 | ATOM | 2961 | CA | PHE | B | 435 | 16.600 | -9.422 | 24.186 | 1.00 | 25.74 |
| | ATOM | 2962 | CB | PHE | B | 435 | 15.278 | -8.972 | 24.825 | 1.00 | 26.53 |
| | ATOM | 2963 | CG | PHE | B | 435 | 14.656 | -7.758 | 24.183 | 1.00 | 30.94 |
| | ATOM | 2964 | CD1 | PHE | B | 435 | 15.118 | -7.271 | 22.966 | 1.00 | 32.65 |
| | ATOM | 2965 | CD2 | PHE | B | 435 | 13.592 | -7.108 | 24.797 | 1.00 | 33.60 |
| 20 | ATOM | 2966 | CE1 | PHE | B | 435 | 14.529 | -6.155 | 22.372 | 1.00 | 36.84 |
| | ATOM | 2967 | CE2 | PHE | B | 435 | 12.997 | -5.989 | 24.208 | 1.00 | 34.96 |
| | ATOM | 2968 | CZ | PHE | B | 435 | 13.468 | -5.516 | 22.995 | 1.00 | 31.64 |
| | ATOM | 2969 | C | PHE | B | 435 | 17.426 | -10.184 | 25.233 | 1.00 | 25.39 |
| | ATOM | 2970 | O | PHE | B | 435 | 18.414 | -9.675 | 25.764 | 1.00 | 22.59 |
| 25 | ATOM | 2971 | N | ARG | B | 436 | 16.999 | -11.405 | 25.528 | 1.00 | 24.58 |
| | ATOM | 2972 | CA | ARG | B | 436 | 17.675 | -12.253 | 26.503 | 1.00 | 30.25 |
| | ATOM | 2973 | CB | ARG | B | 436 | 16.898 | -13.569 | 26.662 | 1.00 | 33.32 |
| | ATOM | 2974 | CG | ARG | B | 436 | 17.232 | -14.358 | 27.915 | 1.00 | 38.17 |
| | ATOM | 2975 | CD | ARG | B | 436 | 16.135 | -15.367 | 28.260 | 1.00 | 37.27 |
| 30 | ATOM | 2976 | NE | ARG | B | 436 | 15.646 | -16.085 | 27.086 | 1.00 | 43.92 |
| | ATOM | 2977 | CZ | ARG | B | 436 | 14.433 | -15.923 | 26.557 | 1.00 | 46.68 |
| | ATOM | 2978 | NH1 | ARG | B | 436 | 13.578 | -15.061 | 27.097 | 1.00 | 45.59 |
| | ATOM | 2979 | NH2 | ARG | B | 436 | 14.074 | -16.620 | 25.486 | 1.00 | 46.25 |
| | ATOM | 2980 | C | ARG | B | 436 | 19.110 | -12.531 | 26.048 | 1.00 | 29.82 |
| 35 | ATOM | 2981 | O | ARG | B | 436 | 20.057 | -12.397 | 26.823 | 1.00 | 28.76 |
| | ATOM | 2982 | N | AMET | B | 437 | 19.269 | -12.921 | 24.789 | 0.50 | 30.27 |
| | ATOM | 2983 | N | BMET | B | 437 | 19.252 | -12.906 | 24.781 | 0.50 | 31.41 |
| | ATOM | 2984 | CA | AMET | B | 437 | 20.591 | -13.212 | 24.253 | 0.50 | 31.98 |
| | ATOM | 2985 | CA | BMET | B | 437 | 20.547 | -13.206 | 24.183 | 0.50 | 33.77 |
| 40 | ATOM | 2986 | CB | AMET | B | 437 | 20.489 | -13.646 | 22.788 | 0.50 | 31.34 |
| | ATOM | 2987 | CB | BMET | B | 437 | 20.348 | -13.595 | 22.714 | 0.50 | 35.88 |
| | ATOM | 2988 | CG | AMET | B | 437 | 20.179 | -15.127 | 22.592 | 0.50 | 33.62 |
| | ATOM | 2989 | CG | BMET | B | 437 | 21.605 | -13.594 | 21.861 | 0.50 | 40.47 |
| | ATOM | 2990 | SD | AMET | B | 437 | 20.354 | -16.099 | 24.109 | 0.50 | 35.21 |
| 45 | ATOM | 2991 | SD | BMET | B | 437 | 21.247 | -13.937 | 20.115 | 0.50 | 46.79 |
| | ATOM | 2992 | CE | AMET | B | 437 | 22.155 | -16.194 | 24.259 | 0.50 | 33.20 |
| | ATOM | 2993 | CE | BMET | B | 437 | 21.837 | -15.632 | 19.976 | 0.50 | 43.22 |
| | ATOM | 2994 | C | AMET | B | 437 | 21.498 | -11.993 | 24.366 | 0.50 | 33.33 |
| | ATOM | 2995 | C | BMET | B | 437 | 21.487 | -12.005 | 24.289 | 0.50 | 34.45 |
| 50 | ATOM | 2996 | O | AMET | B | 437 | 22.702 | -12.123 | 24.594 | 0.50 | 33.54 |
| | ATOM | 2997 | O | BMET | B | 437 | 22.699 | -12.162 | 24.438 | 0.50 | 34.43 |
| | ATOM | 2998 | N | MET | B | 438 | 20.913 | -10.809 | 24.215 | 1.00 | 32.07 |
| | ATOM | 2999 | CA | MET | B | 438 | 21.674 | -9.560 | 24.298 | 1.00 | 32.48 |
| | ATOM | 3000 | CB | MET | B | 438 | 20.930 | -8.437 | 23.578 | 1.00 | 29.74 |
| 55 | ATOM | 3001 | CG | MET | B | 438 | 21.161 | -8.364 | 22.093 | 1.00 | 36.73 |
| | ATOM | 3002 | SD | MET | B | 438 | 20.425 | -6.849 | 21.462 | 1.00 | 38.21 |
| | ATOM | 3003 | CE | MET | B | 438 | 21.693 | -5.657 | 21.943 | 1.00 | 35.91 |
| | ATOM | 3004 | C | MET | B | 438 | 21.877 | -9.122 | 25.738 | 1.00 | 28.81 |
| | ATOM | 3005 | O | MET | B | 438 | 22.686 | -8.240 | 26.013 | 1.00 | 30.13 |
| 60 | ATOM | 3006 | N | ASN | B | 439 | 21.120 | -9.721 | 26.646 | 1.00 | 27.14 |
| | ATOM | 3007 | CA | ASN | B | 439 | 21.199 | -9.359 | 28.038 | 1.00 | 27.34 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3008 | CB | ASN | B | 439 | 22.592 | -9.524 | 28.598 | 1.00 | 34.85 |
| | ATOM | 3009 | CG | ASN | B | 439 | 22.624 | -9.480 | 30.080 | 1.00 | 38.58 |
| | ATOM | 3010 | OD1 | ASN | B | 439 | 21.584 | -9.620 | 30.724 | 1.00 | 42.99 |
| | ATOM | 3011 | ND2 | ASN | B | 439 | 23.801 | -9.260 | 30.666 | 1.00 | 41.14 |
| | ATOM | 3012 | C | ASN | B | 439 | 20.745 | -7.903 | 28.212 | 1.00 | 26.24 |
| 10 | ATOM | 3013 | O | ASN | B | 439 | 21.396 | -7.106 | 28.891 | 1.00 | 19.76 |
| | ATOM | 3014 | N | LEU | B | 440 | 19.625 | -7.564 | 27.573 | 1.00 | 24.90 |
| | ATOM | 3015 | CA | LEU | B | 440 | 19.061 | -6.214 | 27.633 | 1.00 | 25.04 |
| | ATOM | 3016 | CB | LEU | B | 440 | 17.761 | -6.157 | 26.818 | 1.00 | 22.36 |
| | ATOM | 3017 | CG | LEU | B | 440 | 17.087 | -4.786 | 26.740 | 1.00 | 26.33 |
| 15 | ATOM | 3018 | CD1 | LEU | B | 440 | 17.958 | -3.843 | 25.923 | 1.00 | 28.33 |
| | ATOM | 3019 | CD2 | LEU | B | 440 | 15.704 | -4.914 | 26.111 | 1.00 | 24.81 |
| | ATOM | 3020 | C | LEU | B | 440 | 18.782 | -5.785 | 29.074 | 1.00 | 24.71 |
| | ATOM | 3021 | O | LEU | B | 440 | 18.131 | -6.504 | 29.830 | 1.00 | 26.96 |
| | ATOM | 3022 | N | GLN | B | 441 | 19.268 | -4.609 | 29.452 | 1.00 | 25.54 |
| 20 | ATOM | 3023 | CA | GLN | B | 441 | 19.060 | -4.099 | 30.807 | 1.00 | 25.82 |
| | ATOM | 3024 | CB | GLN | B | 441 | 20.250 | -3.231 | 31.234 | 1.00 | 30.41 |
| | ATOM | 3025 | CG | GLN | B | 441 | 21.572 | -3.956 | 31.228 | 1.00 | 30.50 |
| | ATOM | 3026 | CD | GLN | B | 441 | 21.610 | -5.028 | 32.279 | 1.00 | 32.75 |
| | ATOM | 3027 | OE1 | GLN | B | 441 | 21.539 | -4.772 | 33.473 | 1.00 | 36.52 |
| 25 | ATOM | 3028 | NE2 | GLN | B | 441 | 21.703 | -6.288 | 31.823 | 1.00 | 31.09 |
| | ATOM | 3029 | C | GLN | B | 441 | 17.789 | -3.265 | 30.883 | 1.00 | 26.93 |
| | ATOM | 3030 | O | GLN | B | 441 | 17.303 | -2.768 | 29.866 | 1.00 | 25.40 |
| | ATOM | 3031 | N | GLY | B | 442 | 17.266 | -3.105 | 32.096 | 1.00 | 24.56 |
| | ATOM | 3032 | CA | GLY | B | 442 | 16.058 | -2.327 | 32.293 | 1.00 | 22.82 |
| 30 | ATOM | 3033 | C | GLY | B | 442 | 16.217 | -0.873 | 31.885 | 1.00 | 24.19 |
| | ATOM | 3034 | O | GLY | B | 442 | 15.290 | -0.279 | 31.341 | 1.00 | 20.21 |
| | ATOM | 3035 | N | GLU | B | 443 | 17.387 | -0.293 | 32.141 | 1.00 | 22.92 |
| | ATOM | 3036 | CA | GLU | B | 443 | 17.635 | 1.102 | 31.778 | 1.00 | 23.33 |
| | ATOM | 3037 | CB | GLU | B | 443 | 18.960 | 1.590 | 32.378 | 1.00 | 24.26 |
| 35 | ATOM | 3038 | CG | GLU | B | 443 | 19.005 | 1.525 | 33.895 | 1.00 | 32.31 |
| | ATOM | 3039 | CD | GLU | B | 443 | 19.701 | 0.270 | 34.402 | 1.00 | 37.68 |
| | ATOM | 3040 | OE1 | GLU | B | 443 | 19.343 | -0.841 | 33.948 | 1.00 | 35.23 |
| | ATOM | 3041 | OE2 | GLU | B | 443 | 20.607 | 0.394 | 35.252 | 1.00 | 42.47 |
| | ATOM | 3042 | C | GLU | B | 443 | 17.662 | 1.278 | 30.262 | 1.00 | 23.08 |
| 40 | ATOM | 3043 | O | GLU | B | 443 | 17.265 | 2.328 | 29.747 | 1.00 | 21.80 |
| | ATOM | 3044 | N | GLU | B | 444 | 18.128 | 0.253 | 29.552 | 1.00 | 21.16 |
| | ATOM | 3045 | CA | GLU | B | 444 | 18.182 | 0.302 | 28.093 | 1.00 | 22.60 |
| | ATOM | 3046 | CB | GLU | B | 444 | 19.046 | -0.834 | 27.545 | 1.00 | 20.89 |
| | ATOM | 3047 | CG | GLU | B | 444 | 20.545 | -0.617 | 27.705 | 1.00 | 23.24 |
| 45 | ATOM | 3048 | CD | GLU | B | 444 | 21.340 | -1.869 | 27.393 | 1.00 | 22.11 |
| | ATOM | 3049 | OE1 | GLU | B | 444 | 20.817 | -2.978 | 27.629 | 1.00 | 20.89 |
| | ATOM | 3050 | OE2 | GLU | B | 444 | 22.488 | -1.746 | 26.914 | 1.00 | 25.49 |
| | ATOM | 3051 | C | GLU | B | 444 | 16.758 | 0.155 | 27.552 | 1.00 | 21.06 |
| | ATOM | 3052 | O | GLU | B | 444 | 16.377 | 0.822 | 26.597 | 1.00 | 23.73 |
| 50 | ATOM | 3053 | N | PHE | B | 445 | 15.987 | -0.730 | 28.176 | 1.00 | 19.01 |
| | ATOM | 3054 | CA | PHE | B | 445 | 14.600 | -0.969 | 27.792 | 1.00 | 19.44 |
| | ATOM | 3055 | CB | PHE | B | 445 | 13.989 | -2.067 | 28.675 | 1.00 | 18.12 |
| | ATOM | 3056 | CG | PHE | B | 445 | 12.483 | -2.055 | 28.709 | 1.00 | 18.13 |
| | ATOM | 3057 | CD1 | PHE | B | 445 | 11.746 | -2.386 | 27.575 | 1.00 | 18.34 |
| 55 | ATOM | 3058 | CD2 | PHE | B | 445 | 11.802 | -1.694 | 29.872 | 1.00 | 16.59 |
| | ATOM | 3059 | CE1 | PHE | B | 445 | 10.346 | -2.359 | 27.592 | 1.00 | 17.15 |
| | ATOM | 3060 | CE2 | PHE | B | 445 | 10.406 | -1.662 | 29.903 | 1.00 | 21.99 |
| | ATOM | 3061 | CZ | PHE | B | 445 | 9.674 | -1.997 | 28.755 | 1.00 | 16.01 |
| | ATOM | 3062 | C | PHE | B | 445 | 13.758 | 0.304 | 27.888 | 1.00 | 15.87 |
| 60 | ATOM | 3063 | O | PHE | B | 445 | 13.008 | 0.617 | 26.966 | 1.00 | 20.27 |
| | ATOM | 3064 | N | VAL | B | 446 | 13.872 | 1.044 | 28.986 | 1.00 | 15.90 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3065 | CA | VAL | B | 446 | 13.074 | 2.269 | 29.112 | 1.00 | 16.78 |
| | ATOM | 3066 | CB | VAL | B | 446 | 13.165 | 2.895 | 30.531 | 1.00 | 18.32 |
| | ATOM | 3067 | CG1 | VAL | B | 446 | 12.574 | 1.923 | 31.551 | 1.00 | 21.14 |
| | ATOM | 3068 | CG2 | VAL | B | 446 | 14.598 | 3.251 | 30.879 | 1.00 | 21.04 |
| | ATOM | 3069 | C | VAL | B | 446 | 13.450 | 3.295 | 28.051 | 1.00 | 17.91 |
| 10 | ATOM | 3070 | O | VAL | B | 446 | 12.596 | 4.028 | 27.561 | 1.00 | 19.37 |
| | ATOM | 3071 | N | CYS | B | 447 | 14.723 | 3.335 | 27.674 | 1.00 | 18.81 |
| | ATOM | 3072 | CA | CYS | B | 447 | 15.161 | 4.255 | 26.635 | 1.00 | 17.34 |
| | ATOM | 3073 | CB | CYS | B | 447 | 16.682 | 4.224 | 26.512 | 1.00 | 19.33 |
| | ATOM | 3074 | SG | CYS | B | 447 | 17.538 | 5.134 | 27.798 | 1.00 | 23.60 |
| 15 | ATOM | 3075 | C | CYS | B | 447 | 14.537 | 3.826 | 25.301 | 1.00 | 18.09 |
| | ATOM | 3076 | O | CYS | B | 447 | 13.988 | 4.643 | 24.563 | 1.00 | 17.52 |
| | ATOM | 3077 | N | LEU | B | 448 | 14.623 | 2.533 | 25.006 | 1.00 | 15.60 |
| | ATOM | 3078 | CA | LEU | B | 448 | 14.072 | 1.994 | 23.767 | 1.00 | 16.67 |
| | ATOM | 3079 | CB | LEU | B | 448 | 14.328 | 0.490 | 23.684 | 1.00 | 14.82 |
| 20 | ATOM | 3080 | CG | LEU | B | 448 | 15.730 | 0.009 | 23.301 | 1.00 | 23.57 |
| | ATOM | 3081 | CD1 | LEU | B | 448 | 15.722 | -1.522 | 23.169 | 1.00 | 21.61 |
| | ATOM | 3082 | CD2 | LEU | B | 448 | 16.167 | 0.658 | 21.986 | 1.00 | 18.92 |
| | ATOM | 3083 | C | LEU | B | 448 | 12.573 | 2.249 | 23.652 | 1.00 | 15.98 |
| | ATOM | 3084 | O | LEU | B | 448 | 12.078 | 2.633 | 22.590 | 1.00 | 18.91 |
| 25 | ATOM | 3085 | N | LYS | B | 449 | 11.849 | 2.037 | 24.745 | 1.00 | 17.94 |
| | ATOM | 3086 | CA | LYS | B | 449 | 10.405 | 2.232 | 24.733 | 1.00 | 16.66 |
| | ATOM | 3087 | CB | LYS | B | 449 | 9.796 | 1.745 | 26.047 | 1.00 | 16.45 |
| | ATOM | 3088 | CG | LYS | B | 449 | 8.285 | 1.861 | 26.115 | 1.00 | 16.12 |
| | ATOM | 3089 | CD | LYS | B | 449 | 7.730 | 0.952 | 27.193 | 1.00 | 19.09 |
| 30 | ATOM | 3090 | CE | LYS | B | 449 | 8.201 | 1.380 | 28.580 | 1.00 | 17.04 |
| | ATOM | 3091 | NZ | LYS | B | 449 | 7.159 | 1.088 | 29.593 | 1.00 | 17.25 |
| | ATOM | 3092 | C | LYS | B | 449 | 10.058 | 3.696 | 24.486 | 1.00 | 18.78 |
| | ATOM | 3093 | O | LYS | B | 449 | 9.103 | 3.996 | 23.769 | 1.00 | 14.84 |
| | ATOM | 3094 | N | SER | B | 450 | 10.837 | 4.610 | 25.059 | 1.00 | 14.50 |
| 35 | ATOM | 3095 | CA | SER | B | 450 | 10.591 | 6.032 | 24.849 | 1.00 | 17.11 |
| | ATOM | 3096 | CB | SER | B | 450 | 11.440 | 6.866 | 25.815 | 1.00 | 21.20 |
| | ATOM | 3097 | OG | SER | B | 450 | 10.859 | 6.868 | 27.108 | 1.00 | 30.66 |
| | ATOM | 3098 | C | SER | B | 450 | 10.921 | 6.418 | 23.405 | 1.00 | 17.84 |
| | ATOM | 3099 | O | SER | B | 450 | 10.279 | 7.292 | 22.821 | 1.00 | 18.82 |
| 40 | ATOM | 3100 | N | ILE | B | 451 | 11.926 | 5.768 | 22.828 | 1.00 | 16.88 |
| | ATOM | 3101 | CA | ILE | B | 451 | 12.305 | 6.063 | 21.450 | 1.00 | 17.11 |
| | ATOM | 3102 | CB | ILE | B | 451 | 13.564 | 5.268 | 21.025 | 1.00 | 16.69 |
| | ATOM | 3103 | CG2 | ILE | B | 451 | 13.724 | 5.298 | 19.505 | 1.00 | 19.31 |
| | ATOM | 3104 | CG1 | ILE | B | 451 | 14.804 | 5.897 | 21.676 | 1.00 | 18.96 |
| 45 | ATOM | 3105 | CD1 | ILE | B | 451 | 16.083 | 5.130 | 21.431 | 1.00 | 18.98 |
| | ATOM | 3106 | C | ILE | B | 451 | 11.142 | 5.711 | 20.527 | 1.00 | 18.09 |
| | ATOM | 3107 | O | ILE | B | 451 | 10.820 | 6.464 | 19.608 | 1.00 | 17.07 |
| | ATOM | 3108 | N | ILE | B | 452 | 10.505 | 4.571 | 20.786 | 1.00 | 18.13 |
| | ATOM | 3109 | CA | ILE | B | 452 | 9.373 | 4.137 | 19.976 | 1.00 | 16.77 |
| 50 | ATOM | 3110 | CB | ILE | B | 452 | 8.804 | 2.775 | 20.477 | 1.00 | 17.40 |
| | ATOM | 3111 | CG2 | ILE | B | 452 | 7.464 | 2.496 | 19.831 | 1.00 | 14.33 |
| | ATOM | 3112 | CG1 | ILE | B | 452 | 9.763 | 1.635 | 20.107 | 1.00 | 15.36 |
| | ATOM | 3113 | CD1 | ILE | B | 452 | 9.449 | 0.323 | 20.805 | 1.00 | 17.76 |
| | ATOM | 3114 | C | ILE | B | 452 | 8.271 | 5.195 | 20.024 | 1.00 | 17.47 |
| 55 | ATOM | 3115 | O | ILE | B | 452 | 7.733 | 5.586 | 18.992 | 1.00 | 16.50 |
| | ATOM | 3116 | N | LEU | B | 453 | 7.943 | 5.665 | 21.222 | 1.00 | 16.06 |
| | ATOM | 3117 | CA | LEU | B | 453 | 6.903 | 6.680 | 21.374 | 1.00 | 17.17 |
| | ATOM | 3118 | CB | LEU | B | 453 | 6.736 | 7.061 | 22.850 | 1.00 | 16.23 |
| | ATOM | 3119 | CG | LEU | B | 453 | 5.792 | 8.228 | 23.163 | 1.00 | 17.60 |
| 60 | ATOM | 3120 | CD1 | LEU | B | 453 | 4.388 | 7.881 | 22.704 | 1.00 | 16.94 |
| | ATOM | 3121 | CD2 | LEU | B | 453 | 5.816 | 8.538 | 24.667 | 1.00 | 17.17 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3122 | C | LEU | B | 453 | 7.198 | 7.941 | 20.566 | 1.00 | 19.33 |
| | ATOM | 3123 | O | LEU | B | 453 | 6.320 | 8.458 | 19.879 | 1.00 | 21.37 |
| | ATOM | 3124 | N | LEU | B | 454 | 8.434 | 8.428 | 20.636 | 1.00 | 17.68 |
| | ATOM | 3125 | CA | LEU | B | 454 | 8.789 | 9.653 | 19.933 | 1.00 | 20.93 |
| | ATOM | 3126 | CB | LEU | B | 454 | 9.959 | 10.347 | 20.653 | 1.00 | 24.33 |
| 10 | ATOM | 3127 | CG | LEU | B | 454 | 9.735 | 10.699 | 22.130 | 1.00 | 26.16 |
| | ATOM | 3128 | CD1 | LEU | B | 454 | 11.046 | 11.170 | 22.749 | 1.00 | 24.82 |
| | ATOM | 3129 | CD2 | LEU | B | 454 | 8.658 | 11.777 | 22.259 | 1.00 | 23.79 |
| | ATOM | 3130 | C | LEU | B | 454 | 9.120 | 9.494 | 18.449 | 1.00 | 20.75 |
| | ATOM | 3131 | O | LEU | B | 454 | 8.941 | 10.431 | 17.673 | 1.00 | 21.33 |
| 15 | ATOM | 3132 | N | ASN | B | 455 | 9.566 | 8.311 | 18.042 | 1.00 | 20.54 |
| | ATOM | 3133 | CA | ASN | B | 455 | 9.951 | 8.093 | 16.651 | 1.00 | 19.46 |
| | ATOM | 3134 | CB | ASN | B | 455 | 11.147 | 7.149 | 16.584 | 1.00 | 18.58 |
| | ATOM | 3135 | CG | ASN | B | 455 | 11.576 | 6.871 | 15.161 | 1.00 | 17.64 |
| | ATOM | 3136 | OD1 | ASN | B | 455 | 12.106 | 7.749 | 14.496 | 1.00 | 18.40 |
| 20 | ATOM | 3137 | ND2 | ASN | B | 455 | 11.343 | 5.648 | 14.686 | 1.00 | 15.06 |
| | ATOM | 3138 | C | ASN | B | 455 | 8.925 | 7.580 | 15.655 | 1.00 | 22.77 |
| | ATOM | 3139 | O | ASN | B | 455 | 8.790 | 8.127 | 14.564 | 1.00 | 21.94 |
| | ATOM | 3140 | N | SER | B | 456 | 8.224 | 6.514 | 16.023 | 1.00 | 25.90 |
| | ATOM | 3141 | CA | SER | B | 456 | 7.260 | 5.873 | 15.135 | 1.00 | 24.76 |
| 25 | ATOM | 3142 | CB | SER | B | 456 | 6.402 | 4.894 | 15.939 | 1.00 | 26.91 |
| | ATOM | 3143 | OG | SER | B | 456 | 7.212 | 3.818 | 16.390 | 1.00 | 26.24 |
| | ATOM | 3144 | C | SER | B | 456 | 6.385 | 6.774 | 14.272 | 1.00 | 26.52 |
| | ATOM | 3145 | O | SER | B | 456 | 6.323 | 6.588 | 13.055 | 1.00 | 29.22 |
| | ATOM | 3146 | N | GLY | B | 457 | 5.716 | 7.750 | 14.872 | 1.00 | 22.07 |
| 30 | ATOM | 3147 | CA | GLY | B | 457 | 4.879 | 8.627 | 14.076 | 1.00 | 25.19 |
| | ATOM | 3148 | C | GLY | B | 457 | 5.510 | 9.973 | 13.765 | 1.00 | 28.59 |
| | ATOM | 3149 | O | GLY | B | 457 | 4.851 | 10.850 | 13.214 | 1.00 | 28.31 |
| | ATOM | 3150 | N | VAL | B | 458 | 6.789 | 10.130 | 14.092 | 1.00 | 31.65 |
| | ATOM | 3151 | CA | VAL | B | 458 | 7.486 | 11.396 | 13.879 | 1.00 | 38.50 |
| 35 | ATOM | 3152 | CB | VAL | B | 458 | 8.950 | 11.310 | 14.373 | 1.00 | 36.24 |
| | ATOM | 3153 | CG1 | VAL | B | 458 | 9.827 | 10.650 | 13.324 | 1.00 | 38.50 |
| | ATOM | 3154 | CG2 | VAL | B | 458 | 9.463 | 12.699 | 14.701 | 1.00 | 39.84 |
| | ATOM | 3155 | C | VAL | B | 458 | 7.483 | 11.982 | 12.464 | 1.00 | 46.30 |
| | ATOM | 3156 | O | VAL | B | 458 | 7.567 | 13.201 | 12.302 | 1.00 | 47.67 |
| 40 | ATOM | 3157 | N | TYR | B | 459 | 7.393 | 11.138 | 11.442 | 1.00 | 50.45 |
| | ATOM | 3158 | CA | TYR | B | 459 | 7.385 | 11.640 | 10.069 | 1.00 | 57.07 |
| | ATOM | 3159 | CB | TYR | B | 459 | 8.233 | 10.740 | 9.170 | 1.00 | 57.05 |
| | ATOM | 3160 | CG | TYR | B | 459 | 9.673 | 10.680 | 9.611 | 1.00 | 59.29 |
| | ATOM | 3161 | CD1 | TYR | B | 459 | 10.284 | 11.786 | 10.203 | 1.00 | 60.93 |
| 45 | ATOM | 3162 | CE1 | TYR | B | 459 | 11.591 | 11.725 | 10.662 | 1.00 | 61.86 |
| | ATOM | 3163 | CD2 | TYR | B | 459 | 10.414 | 9.510 | 9.486 | 1.00 | 59.46 |
| | ATOM | 3164 | CE2 | TYR | B | 459 | 11.726 | 9.439 | 9.943 | 1.00 | 59.67 |
| | ATOM | 3165 | CZ | TYR | B | 459 | 12.305 | 10.548 | 10.532 | 1.00 | 60.84 |
| | ATOM | 3166 | OH | TYR | B | 459 | 13.593 | 10.477 | 11.009 | 1.00 | 61.39 |
| 50 | ATOM | 3167 | C | TYR | B | 459 | 5.976 | 11.753 | 9.514 | 1.00 | 61.22 |
| | ATOM | 3168 | O | TYR | B | 459 | 5.629 | 12.750 | 8.874 | 1.00 | 62.89 |
| | ATOM | 3169 | N | THR | B | 460 | 5.166 | 10.730 | 9.768 | 1.00 | 65.15 |
| | ATOM | 3170 | CA | THR | B | 460 | 3.783 | 10.702 | 9.309 | 1.00 | 67.76 |
| | ATOM | 3171 | CB | THR | B | 460 | 3.178 | 9.283 | 9.464 | 1.00 | 68.02 |
| 55 | ATOM | 3172 | OG1 | THR | B | 460 | 1.890 | 9.235 | 8.836 | 1.00 | 67.03 |
| | ATOM | 3173 | CG2 | THR | B | 460 | 3.040 | 8.916 | 10.938 | 1.00 | 67.31 |
| | ATOM | 3174 | C | THR | B | 460 | 2.945 | 11.700 | 10.107 | 1.00 | 70.14 |
| | ATOM | 3175 | O | THR | B | 460 | 1.715 | 11.641 | 10.099 | 1.00 | 72.35 |
| | ATOM | 3176 | N | PHE | B | 461 | 3.625 | 12.620 | 10.788 | 1.00 | 72.64 |
| 60 | ATOM | 3177 | CA | PHE | B | 461 | 2.969 | 13.637 | 11.607 | 1.00 | 75.05 |
| | ATOM | 3178 | CB | PHE | B | 461 | 3.977 | 14.720 | 12.012 | 1.00 | 75.47 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3179 | CG | PHE | B | 461 | 4.235 | 14.789 | 13.492 | 1.00 | 74.32 |
| | ATOM | 3180 | CD1 | PHE | B | 461 | 3.200 | 14.609 | 14.404 | 1.00 | 73.98 |
| | ATOM | 3181 | CD2 | PHE | B | 461 | 5.517 | 15.025 | 13.975 | 1.00 | 75.22 |
| | ATOM | 3182 | CE1 | PHE | B | 461 | 3.438 | 14.662 | 15.775 | 1.00 | 74.02 |
| | ATOM | 3183 | CE2 | PHE | B | 461 | 5.765 | 15.080 | 15.344 | 1.00 | 74.50 |
| 10 | ATOM | 3184 | CZ | PHE | B | 461 | 4.722 | 14.897 | 16.245 | 1.00 | 74.10 |
| | ATOM | 3185 | C | PHE | B | 461 | 1.787 | 14.286 | 10.896 | 1.00 | 76.78 |
| | ATOM | 3186 | O | PHE | B | 461 | 1.775 | 14.279 | 9.645 | 1.00 | 77.08 |
| | ATOM | 3187 | CB | GLU | B | 470 | 7.873 | 23.789 | 14.718 | 1.00 | 80.19 |
| | ATOM | 3188 | C | GLU | B | 470 | 8.958 | 21.731 | 15.650 | 1.00 | 79.30 |
| 15 | ATOM | 3189 | O | GLU | B | 470 | 9.887 | 21.518 | 16.432 | 1.00 | 78.21 |
| | ATOM | 3190 | N | GLU | B | 470 | 9.096 | 22.235 | 13.227 | 1.00 | 80.22 |
| | ATOM | 3191 | CA | GLU | B | 470 | 9.060 | 22.830 | 14.595 | 1.00 | 80.03 |
| | ATOM | 3192 | N | GLU | B | 471 | 7.823 | 21.037 | 15.665 | 1.00 | 78.31 |
| | ATOM | 3193 | CA | GLU | B | 471 | 7.596 | 19.956 | 16.617 | 1.00 | 75.83 |
| 20 | ATOM | 3194 | CB | GLU | B | 471 | 6.118 | 19.543 | 16.604 | 1.00 | 76.70 |
| | ATOM | 3195 | CG | GLU | B | 471 | 5.742 | 18.544 | 15.516 | 1.00 | 78.42 |
| | ATOM | 3196 | CD | GLU | B | 471 | 5.062 | 19.198 | 14.327 | 1.00 | 79.69 |
| | ATOM | 3197 | OE1 | GLU | B | 471 | 3.829 | 19.398 | 14.378 | 1.00 | 80.26 |
| | ATOM | 3198 | OE2 | GLU | B | 471 | 5.763 | 19.511 | 13.340 | 1.00 | 80.72 |
| 25 | ATOM | 3199 | C | GLU | B | 471 | 8.487 | 18.756 | 16.292 | 1.00 | 73.13 |
| | ATOM | 3200 | O | GLU | B | 471 | 8.897 | 18.021 | 17.189 | 1.00 | 73.86 |
| | ATOM | 3201 | N | LYS | B | 472 | 8.785 | 18.565 | 15.009 | 1.00 | 69.65 |
| | ATOM | 3202 | CA | LYS | B | 472 | 9.639 | 17.461 | 14.581 | 1.00 | 64.40 |
| | ATOM | 3203 | CB | LYS | B | 472 | 9.578 | 17.293 | 13.060 | 1.00 | 63.78 |
| 30 | ATOM | 3204 | CG | LYS | B | 472 | 8.343 | 16.552 | 12.566 | 1.00 | 64.49 |
| | ATOM | 3205 | CD | LYS | B | 472 | 8.544 | 16.002 | 11.161 | 1.00 | 63.81 |
| | ATOM | 3206 | CE | LYS | B | 472 | 7.379 | 16.368 | 10.249 | 1.00 | 64.90 |
| | ATOM | 3207 | NZ | LYS | B | 472 | 6.475 | 15.212 | 9.990 | 1.00 | 63.97 |
| | ATOM | 3208 | C | LYS | B | 472 | 11.071 | 17.749 | 15.014 | 1.00 | 61.03 |
| 35 | ATOM | 3209 | O | LYS | B | 472 | 11.848 | 16.833 | 15.287 | 1.00 | 60.28 |
| | ATOM | 3210 | N | ASP | B | 473 | 11.413 | 19.033 | 15.076 | 1.00 | 56.84 |
| | ATOM | 3211 | CA | ASP | B | 473 | 12.745 | 19.451 | 15.488 | 1.00 | 51.69 |
| | ATOM | 3212 | CB | ASP | B | 473 | 12.923 | 20.940 | 15.242 | 1.00 | 50.36 |
| | ATOM | 3213 | C | ASP | B | 473 | 12.923 | 19.138 | 16.970 | 1.00 | 49.18 |
| 40 | ATOM | 3214 | O | ASP | B | 473 | 13.959 | 18.619 | 17.385 | 1.00 | 46.85 |
| | ATOM | 3215 | N | HIS | B | 474 | 11.898 | 19.449 | 17.758 | 1.00 | 45.35 |
| | ATOM | 3216 | CA | HIS | B | 474 | 11.923 | 19.203 | 19.196 | 1.00 | 43.65 |
| | ATOM | 3217 | CB | HIS | B | 474 | 10.652 | 19.761 | 19.847 | 1.00 | 43.70 |
| | ATOM | 3218 | CG | HIS | B | 474 | 10.458 | 19.326 | 21.267 | 1.00 | 43.86 |
| 45 | ATOM | 3219 | CD2 | HIS | B | 474 | 11.095 | 19.688 | 22.406 | 1.00 | 44.12 |
| | ATOM | 3220 | ND1 | HIS | B | 474 | 9.510 | 18.395 | 21.638 | 1.00 | 46.60 |
| | ATOM | 3221 | CE1 | HIS | B | 474 | 9.572 | 18.202 | 22.943 | 1.00 | 45.29 |
| | ATOM | 3222 | NE2 | HIS | B | 474 | 10.526 | 18.975 | 23.434 | 1.00 | 47.96 |
| | ATOM | 3223 | C | HIS | B | 474 | 12.030 | 17.707 | 19.471 | 1.00 | 42.38 |
| 50 | ATOM | 3224 | O | HIS | B | 474 | 12.834 | 17.273 | 20.298 | 1.00 | 42.83 |
| | ATOM | 3225 | N | ILE | B | 475 | 11.214 | 16.923 | 18.773 | 1.00 | 38.86 |
| | ATOM | 3226 | CA | ILE | B | 475 | 11.222 | 15.475 | 18.943 | 1.00 | 36.53 |
| | ATOM | 3227 | CB | ILE | B | 475 | 10.105 | 14.822 | 18.110 | 1.00 | 36.56 |
| | ATOM | 3228 | CG2 | ILE | B | 475 | 10.390 | 13.335 | 17.911 | 1.00 | 36.17 |
| 55 | ATOM | 3229 | CG1 | ILE | B | 475 | 8.770 | 14.998 | 18.832 | 1.00 | 35.81 |
| | ATOM | 3230 | CD1 | ILE | B | 475 | 7.598 | 14.410 | 18.094 | 1.00 | 41.77 |
| | ATOM | 3231 | C | ILE | B | 475 | 12.575 | 14.898 | 18.532 | 1.00 | 33.72 |
| | ATOM | 3232 | O | ILE | B | 475 | 13.112 | 14.023 | 19.207 | 1.00 | 31.50 |
| | ATOM | 3233 | N | HIS | B | 476 | 13.121 | 15.375 | 17.429 | 1.00 | 33.65 |
| 60 | ATOM | 3234 | CA | HIS | B | 476 | 14.421 | 14.886 | 16.992 | 1.00 | 33.31 |
| | ATOM | 3235 | CB | HIS | B | 476 | 14.782 | 15.481 | 15.637 | 1.00 | 37.30 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3236 | CG | HIS | B | 476 | 14.132 | 14.781 | 14.486 | 1.00 | 43.64 |
| | ATOM | 3237 | CD2 | HIS | B | 476 | 13.723 | 13.498 | 14.342 | 1.00 | 45.25 |
| | ATOM | 3238 | ND1 | HIS | B | 476 | 13.816 | 15.419 | 13.306 | 1.00 | 48.37 |
| | ATOM | 3239 | CE1 | HIS | B | 476 | 13.238 | 14.560 | 12.484 | 1.00 | 48.87 |
| | ATOM | 3240 | NE2 | HIS | B | 476 | 13.170 | 13.387 | 13.089 | 1.00 | 48.11 |
| 10 | ATOM | 3241 | C | HIS | B | 476 | 15.506 | 15.213 | 18.022 | 1.00 | 31.20 |
| | ATOM | 3242 | O | HIS | B | 476 | 16.442 | 14.436 | 18.208 | 1.00 | 27.25 |
| | ATOM | 3243 | N | ARG | B | 477 | 15.387 | 16.365 | 18.684 | 1.00 | 30.64 |
| | ATOM | 3244 | CA | ARG | B | 477 | 16.361 | 16.754 | 19.703 | 1.00 | 30.09 |
| | ATOM | 3245 | CB | ARG | B | 477 | 16.144 | 18.214 | 20.121 | 1.00 | 33.46 |
| 15 | ATOM | 3246 | CG | ARG | B | 477 | 16.322 | 19.212 | 18.982 | 1.00 | 40.74 |
| | ATOM | 3247 | CD | ARG | B | 477 | 16.274 | 20.649 | 19.479 | 1.00 | 45.91 |
| | ATOM | 3248 | NE | ARG | B | 477 | 17.514 | 21.020 | 20.155 | 1.00 | 51.37 |
| | ATOM | 3249 | CZ | ARG | B | 477 | 18.375 | 21.927 | 19.702 | 1.00 | 53.68 |
| | ATOM | 3250 | NH1 | ARG | B | 477 | 18.140 | 22.567 | 18.560 | 1.00 | 53.04 |
| 20 | ATOM | 3251 | NH2 | ARG | B | 477 | 19.480 | 22.185 | 20.389 | 1.00 | 51.79 |
| | ATOM | 3252 | C | ARG | B | 477 | 16.232 | 15.835 | 20.925 | 1.00 | 26.97 |
| | ATOM | 3253 | O | ARG | B | 477 | 17.233 | 15.387 | 21.486 | 1.00 | 27.34 |
| | ATOM | 3254 | N | VAL | B | 478 | 14.999 | 15.558 | 21.338 | 1.00 | 23.70 |
| | ATOM | 3255 | CA | VAL | B | 478 | 14.780 | 14.685 | 22.482 | 1.00 | 24.79 |
| 25 | ATOM | 3256 | CB | VAL | B | 478 | 13.286 | 14.613 | 22.861 | 1.00 | 24.83 |
| | ATOM | 3257 | CG1 | VAL | B | 478 | 13.088 | 13.646 | 24.022 | 1.00 | 26.23 |
| | ATOM | 3258 | CG2 | VAL | B | 478 | 12.781 | 15.996 | 23.243 | 1.00 | 28.26 |
| | ATOM | 3259 | C | VAL | B | 478 | 15.284 | 13.294 | 22.112 | 1.00 | 26.10 |
| | ATOM | 3260 | O | VAL | B | 478 | 15.919 | 12.613 | 22.927 | 1.00 | 24.28 |
| 30 | ATOM | 3261 | N | LEU | B | 479 | 15.021 | 12.889 | 20.870 | 1.00 | 22.92 |
| | ATOM | 3262 | CA | LEU | B | 479 | 15.456 | 11.584 | 20.379 | 1.00 | 21.96 |
| | ATOM | 3263 | CB | LEU | B | 479 | 14.992 | 11.372 | 18.930 | 1.00 | 22.63 |
| | ATOM | 3264 | CG | LEU | B | 479 | 13.575 | 10.798 | 18.756 | 1.00 | 20.82 |
| | ATOM | 3265 | CD1 | LEU | B | 479 | 13.231 | 10.689 | 17.274 | 1.00 | 22.53 |
| 35 | ATOM | 3266 | CD2 | LEU | B | 479 | 13.495 | 9.440 | 19.420 | 1.00 | 23.08 |
| | ATOM | 3267 | C | LEU | B | 479 | 16.975 | 11.471 | 20.453 | 1.00 | 21.90 |
| | ATOM | 3268 | O | LEU | B | 479 | 17.506 | 10.416 | 20.778 | 1.00 | 23.11 |
| | ATOM | 3269 | N | ASP | B | 480 | 17.675 | 12.560 | 20.143 | 1.00 | 23.65 |
| | ATOM | 3270 | CA | ASP | B | 480 | 19.141 | 12.566 | 20.198 | 1.00 | 24.29 |
| 40 | ATOM | 3271 | CB | ASP | B | 480 | 19.692 | 13.889 | 19.649 | 1.00 | 26.88 |
| | ATOM | 3272 | CG | ASP | B | 480 | 19.773 | 13.914 | 18.129 | 1.00 | 33.32 |
| | ATOM | 3273 | OD1 | ASP | B | 480 | 19.857 | 12.836 | 17.499 | 1.00 | 35.44 |
| | ATOM | 3274 | OD2 | ASP | B | 480 | 19.757 | 15.022 | 17.563 | 1.00 | 32.44 |
| | ATOM | 3275 | C | ASP | B | 480 | 19.590 | 12.406 | 21.656 | 1.00 | 24.13 |
| 45 | ATOM | 3276 | O | ASP | B | 480 | 20.551 | 11.697 | 21.956 | 1.00 | 24.88 |
| | ATOM | 3277 | N | LYS | B | 481 | 18.887 | 13.077 | 22.560 | 1.00 | 25.18 |
| | ATOM | 3278 | CA | LYS | B | 481 | 19.213 | 13.010 | 23.980 | 1.00 | 26.78 |
| | ATOM | 3279 | CB | LYS | B | 481 | 18.262 | 13.898 | 24.785 | 1.00 | 31.37 |
| | ATOM | 3280 | CG | LYS | B | 481 | 18.962 | 14.788 | 25.804 | 1.00 | 43.84 |
| 50 | ATOM | 3281 | CD | LYS | B | 481 | 18.780 | 14.260 | 27.219 | 1.00 | 46.08 |
| | ATOM | 3282 | CE | LYS | B | 481 | 20.120 | 13.928 | 27.865 | 1.00 | 50.99 |
| | ATOM | 3283 | NZ | LYS | B | 481 | 21.177 | 14.922 | 27.511 | 1.00 | 54.35 |
| | ATOM | 3284 | C | LYS | B | 481 | 19.124 | 11.575 | 24.495 | 1.00 | 26.87 |
| | ATOM | 3285 | O | LYS | B | 481 | 19.951 | 11.145 | 25.305 | 1.00 | 20.37 |
| 55 | ATOM | 3286 | N | ILE | B | 482 | 18.124 | 10.830 | 24.027 | 1.00 | 23.26 |
| | ATOM | 3287 | CA | ILE | B | 482 | 17.981 | 9.452 | 24.472 | 1.00 | 21.07 |
| | ATOM | 3288 | CB | ILE | B | 482 | 16.655 | 8.828 | 24.015 | 1.00 | 19.80 |
| | ATOM | 3289 | CG2 | ILE | B | 482 | 16.580 | 7.370 | 24.491 | 1.00 | 17.40 |
| | ATOM | 3290 | CG1 | ILE | B | 482 | 15.479 | 9.606 | 24.602 | 1.00 | 17.16 |
| 60 | ATOM | 3291 | CD1 | ILE | B | 482 | 14.136 | 9.209 | 23.991 | 1.00 | 19.43 |
| | ATOM | 3292 | C | ILE | B | 482 | 19.135 | 8.616 | 23.947 | 1.00 | 20.21 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3293 | O | ILE | B | 482 | 19.621 | 7.722 | 24.640 | 1.00 | 25.55 |
| | ATOM | 3294 | N | THR | B | 483 | 19.569 | 8.896 | 22.722 | 1.00 | 21.89 |
| | ATOM | 3295 | CA | THR | B | 483 | 20.701 | 8.176 | 22.141 | 1.00 | 22.67 |
| | ATOM | 3296 | CB | THR | B | 483 | 21.030 | 8.662 | 20.695 | 1.00 | 23.34 |
| | ATOM | 3297 | OG1 | THR | B | 483 | 19.890 | 8.475 | 19.851 | 1.00 | 27.33 |
| 10 | ATOM | 3298 | CG2 | THR | B | 483 | 22.203 | 7.882 | 20.116 | 1.00 | 24.46 |
| | ATOM | 3299 | C | THR | B | 483 | 21.913 | 8.441 | 23.035 | 1.00 | 23.51 |
| | ATOM | 3300 | O | THR | B | 483 | 22.650 | 7.520 | 23.381 | 1.00 | 27.01 |
| | ATOM | 3301 | N | ASP | B | 484 | 22.119 | 9.703 | 23.404 | 1.00 | 22.88 |
| | ATOM | 3302 | CA | ASP | B | 484 | 23.237 | 10.058 | 24.276 | 1.00 | 24.93 |
| 15 | ATOM | 3303 | CB | ASP | B | 484 | 23.201 | 11.546 | 24.652 | 1.00 | 28.69 |
| | ATOM | 3304 | CG | ASP | B | 484 | 23.504 | 12.464 | 23.485 | 1.00 | 29.19 |
| | ATOM | 3305 | OD1 | ASP | B | 484 | 23.982 | 11.984 | 22.437 | 1.00 | 29.63 |
| | ATOM | 3306 | OD2 | ASP | B | 484 | 23.256 | 13.681 | 23.627 | 1.00 | 32.02 |
| | ATOM | 3307 | C | ASP | B | 484 | 23.125 | 9.249 | 25.567 | 1.00 | 24.40 |
| 20 | ATOM | 3308 | O | ASP | B | 484 | 24.125 | 8.780 | 26.103 | 1.00 | 25.60 |
| | ATOM | 3309 | N | THR | B | 485 | 21.899 | 9.096 | 26.066 | 1.00 | 20.16 |
| | ATOM | 3310 | CA | THR | B | 485 | 21.670 | 8.365 | 27.307 | 1.00 | 22.28 |
| | ATOM | 3311 | CB | THR | B | 485 | 20.203 | 8.521 | 27.763 | 1.00 | 24.64 |
| | ATOM | 3312 | OG1 | THR | B | 485 | 19.878 | 9.914 | 27.830 | 1.00 | 24.28 |
| 25 | ATOM | 3313 | CG2 | THR | B | 485 | 19.993 | 7.896 | 29.133 | 1.00 | 23.32 |
| | ATOM | 3314 | C | THR | B | 485 | 22.017 | 6.881 | 27.188 | 1.00 | 22.13 |
| | ATOM | 3315 | O | THR | B | 485 | 22.574 | 6.284 | 28.115 | 1.00 | 23.30 |
| | ATOM | 3316 | N | LEU | B | 486 | 21.686 | 6.290 | 26.045 | 1.00 | 23.08 |
| | ATOM | 3317 | CA | LEU | B | 486 | 21.969 | 4.881 | 25.792 | 1.00 | 22.26 |
| 30 | ATOM | 3318 | CB | LEU | B | 486 | 21.346 | 4.452 | 24.464 | 1.00 | 20.93 |
| | ATOM | 3319 | CG | LEU | B | 486 | 19.878 | 4.031 | 24.533 | 1.00 | 24.92 |
| | ATOM | 3320 | CD1 | LEU | B | 486 | 19.295 | 4.003 | 23.123 | 1.00 | 21.96 |
| | ATOM | 3321 | CD2 | LEU | B | 486 | 19.763 | 2.658 | 25.196 | 1.00 | 23.90 |
| | ATOM | 3322 | C | LEU | B | 486 | 23.477 | 4.634 | 25.742 | 1.00 | 24.12 |
| 35 | ATOM | 3323 | O | LEU | B | 486 | 23.984 | 3.681 | 26.334 | 1.00 | 24.02 |
| | ATOM | 3324 | N | ILE | B | 487 | 24.191 | 5.490 | 25.022 | 1.00 | 24.53 |
| | ATOM | 3325 | CA | ILE | B | 487 | 25.640 | 5.345 | 24.913 | 1.00 | 25.16 |
| | ATOM | 3326 | CB | ILE | B | 487 | 26.207 | 6.379 | 23.899 | 1.00 | 25.57 |
| | ATOM | 3327 | CG2 | ILE | B | 487 | 27.725 | 6.522 | 24.051 | 1.00 | 24.54 |
| 40 | ATOM | 3328 | CG1 | ILE | B | 487 | 25.857 | 5.936 | 22.470 | 1.00 | 25.63 |
| | ATOM | 3329 | CD1 | ILE | B | 487 | 26.538 | 4.646 | 22.021 | 1.00 | 25.68 |
| | ATOM | 3330 | C | ILE | B | 487 | 26.275 | 5.518 | 26.307 | 1.00 | 23.60 |
| | ATOM | 3331 | O | ILE | B | 487 | 27.200 | 4.794 | 26.671 | 1.00 | 23.65 |
| | ATOM | 3332 | N | HIS | B | 488 | 25.755 | 6.456 | 27.081 | 1.00 | 21.75 |
| 45 | ATOM | 3333 | CA | HIS | B | 488 | 26.251 | 6.720 | 28.431 | 1.00 | 26.07 |
| | ATOM | 3334 | CB | HIS | B | 488 | 25.450 | 7.871 | 29.041 | 1.00 | 26.99 |
| | ATOM | 3335 | CG | HIS | B | 488 | 25.818 | 8.196 | 30.455 | 1.00 | 33.06 |
| | ATOM | 3336 | CD2 | HIS | B | 488 | 25.245 | 7.838 | 31.629 | 1.00 | 32.79 |
| | ATOM | 3337 | ND1 | HIS | B | 488 | 26.869 | 9.025 | 30.779 | 1.00 | 36.45 |
| 50 | ATOM | 3338 | CE1 | HIS | B | 488 | 26.927 | 9.164 | 32.091 | 1.00 | 35.93 |
| | ATOM | 3339 | NE2 | HIS | B | 488 | 25.953 | 8.453 | 32.630 | 1.00 | 33.88 |
| | ATOM | 3340 | C | HIS | B | 488 | 26.123 | 5.463 | 29.292 | 1.00 | 26.85 |
| | ATOM | 3341 | O | HIS | B | 488 | 27.071 | 5.054 | 29.967 | 1.00 | 28.52 |
| | ATOM | 3342 | N | LEU | B | 489 | 24.949 | 4.850 | 29.266 | 1.00 | 28.00 |
| 55 | ATOM | 3343 | CA | LEU | B | 489 | 24.715 | 3.642 | 30.040 | 1.00 | 25.94 |
| | ATOM | 3344 | CB | LEU | B | 489 | 23.298 | 3.127 | 29.788 | 1.00 | 27.07 |
| | ATOM | 3345 | CG | LEU | B | 489 | 22.158 | 3.909 | 30.445 | 1.00 | 31.71 |
| | ATOM | 3346 | CD1 | LEU | B | 489 | 20.827 | 3.516 | 29.799 | 1.00 | 28.08 |
| | ATOM | 3347 | CD2 | LEU | B | 489 | 22.143 | 3.616 | 31.949 | 1.00 | 29.30 |
| 60 | ATOM | 3348 | C | LEU | B | 489 | 25.718 | 2.561 | 29.642 | 1.00 | 26.84 |
| | ATOM | 3349 | O | LEU | B | 489 | 26.241 | 1.832 | 30.486 | 1.00 | 20.86 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3350 | N | MET | B | 490 | 25.978 | 2.453 | 28.345 | 1.00 | 23.82 |
| | ATOM | 3351 | CA | MET | B | 490 | 26.900 | 1.438 | 27.857 | 1.00 | 26.38 |
| | ATOM | 3352 | CB | MET | B | 490 | 26.775 | 1.306 | 26.336 | 1.00 | 27.29 |
| | ATOM | 3353 | CG | MET | B | 490 | 25.418 | 0.776 | 25.895 | 1.00 | 21.68 |
| | ATOM | 3354 | SD | MET | B | 490 | 25.208 | 0.739 | 24.106 | 1.00 | 26.30 |
| 10 | ATOM | 3355 | CE | MET | B | 490 | 23.461 | 0.412 | 24.022 | 1.00 | 19.66 |
| | ATOM | 3356 | C | MET | B | 490 | 28.341 | 1.743 | 28.247 | 1.00 | 26.42 |
| | ATOM | 3357 | O | MET | B | 490 | 29.109 | 0.833 | 28.574 | 1.00 | 24.76 |
| | ATOM | 3358 | N | ALA | B | 491 | 28.713 | 3.018 | 28.207 | 1.00 | 26.67 |
| | ATOM | 3359 | CA | ALA | B | 491 | 30.074 | 3.394 | 28.577 | 1.00 | 30.73 |
| 15 | ATOM | 3360 | CB | ALA | B | 491 | 30.299 | 4.882 | 28.335 | 1.00 | 26.66 |
| | ATOM | 3361 | C | ALA | B | 491 | 30.250 | 3.053 | 30.056 | 1.00 | 32.08 |
| | ATOM | 3362 | O | ALA | B | 491 | 31.194 | 2.361 | 30.438 | 1.00 | 34.66 |
| | ATOM | 3363 | N | LYS | B | 492 | 29.316 | 3.523 | 30.878 | 1.00 | 33.17 |
| | ATOM | 3364 | CA | LYS | B | 492 | 29.354 | 3.267 | 32.309 | 1.00 | 32.82 |
| 20 | ATOM | 3365 | CB | LYS | B | 492 | 28.110 | 3.849 | 32.976 | 1.00 | 36.38 |
| | ATOM | 3366 | CG | LYS | B | 492 | 28.412 | 4.797 | 34.123 | 1.00 | 38.68 |
| | ATOM | 3367 | CD | LYS | B | 492 | 27.242 | 4.887 | 35.084 | 1.00 | 41.41 |
| | ATOM | 3368 | CE | LYS | B | 492 | 26.299 | 6.013 | 34.698 | 1.00 | 47.57 |
| | ATOM | 3369 | NZ | LYS | B | 492 | 26.395 | 7.184 | 35.618 | 1.00 | 50.76 |
| 25 | ATOM | 3370 | C | LYS | B | 492 | 29.453 | 1.771 | 32.619 | 1.00 | 34.08 |
| | ATOM | 3371 | O | LYS | B | 492 | 30.090 | 1.382 | 33.593 | 1.00 | 34.31 |
| | ATOM | 3372 | N | ALA | B | 493 | 28.835 | 0.935 | 31.788 | 1.00 | 32.03 |
| | ATOM | 3373 | CA | ALA | B | 493 | 28.867 | -0.510 | 31.998 | 1.00 | 30.70 |
| | ATOM | 3374 | CB | ALA | B | 493 | 27.719 | -1.181 | 31.245 | 1.00 | 28.80 |
| 30 | ATOM | 3375 | C | ALA | B | 493 | 30.201 | -1.156 | 31.606 | 1.00 | 33.75 |
| | ATOM | 3376 | O | ALA | B | 493 | 30.402 | -2.356 | 31.819 | 1.00 | 30.53 |
| | ATOM | 3377 | N | GLY | B | 494 | 31.102 | -0.372 | 31.020 | 1.00 | 33.50 |
| | ATOM | 3378 | CA | GLY | B | 494 | 32.405 | -0.903 | 30.656 | 1.00 | 33.71 |
| | ATOM | 3379 | C | GLY | B | 494 | 32.639 | -1.360 | 29.230 | 1.00 | 34.40 |
| 35 | ATOM | 3380 | O | GLY | B | 494 | 33.663 | -1.989 | 28.950 | 1.00 | 33.13 |
| | ATOM | 3381 | N | LEU | B | 495 | 31.712 | -1.056 | 28.326 | 1.00 | 31.76 |
| | ATOM | 3382 | CA | LEU | B | 495 | 31.859 | -1.452 | 26.925 | 1.00 | 30.57 |
| | ATOM | 3383 | CB | LEU | B | 495 | 30.494 | -1.415 | 26.216 | 1.00 | 30.67 |
| | ATOM | 3384 | CG | LEU | B | 495 | 29.610 | -2.675 | 26.256 | 1.00 | 29.59 |
| 40 | ATOM | 3385 | CD1 | LEU | B | 495 | 29.315 | -3.058 | 27.700 | 1.00 | 26.60 |
| | ATOM | 3386 | CD2 | LEU | B | 495 | 28.307 | -2.416 | 25.501 | 1.00 | 27.52 |
| | ATOM | 3387 | C | LEU | B | 495 | 32.829 | -0.515 | 26.202 | 1.00 | 30.53 |
| | ATOM | 3388 | O | LEU | B | 495 | 32.855 | 0.688 | 26.468 | 1.00 | 28.14 |
| | ATOM | 3389 | N | THR | B | 496 | 33.628 | -1.064 | 25.291 | 1.00 | 28.03 |
| 45 | ATOM | 3390 | CA | THR | B | 496 | 34.567 | -0.243 | 24.529 | 1.00 | 29.06 |
| | ATOM | 3391 | CB | THR | B | 496 | 35.511 | -1.095 | 23.665 | 1.00 | 29.40 |
| | ATOM | 3392 | OG1 | THR | B | 496 | 34.753 | -1.758 | 22.641 | 1.00 | 30.29 |
| | ATOM | 3393 | CG2 | THR | B | 496 | 36.228 | -2.122 | 24.515 | 1.00 | 28.12 |
| | ATOM | 3394 | C | THR | B | 496 | 33.770 | 0.652 | 23.590 | 1.00 | 30.12 |
| 50 | ATOM | 3395 | O | THR | B | 496 | 32.580 | 0.433 | 23.380 | 1.00 | 29.74 |
| | ATOM | 3396 | N | LEU | B | 497 | 34.430 | 1.654 | 23.018 | 1.00 | 30.44 |
| | ATOM | 3397 | CA | LEU | B | 497 | 33.762 | 2.567 | 22.104 | 1.00 | 28.54 |
| | ATOM | 3398 | CB | LEU | B | 497 | 34.768 | 3.564 | 21.529 | 1.00 | 31.14 |
| | ATOM | 3399 | CG | LEU | B | 497 | 35.209 | 4.719 | 22.434 | 1.00 | 33.58 |
| 55 | ATOM | 3400 | CD1 | LEU | B | 497 | 36.120 | 5.659 | 21.652 | 1.00 | 31.42 |
| | ATOM | 3401 | CD2 | LEU | B | 497 | 33.992 | 5.469 | 22.942 | 1.00 | 35.08 |
| | ATOM | 3402 | C | LEU | B | 497 | 33.095 | 1.800 | 20.967 | 1.00 | 27.35 |
| | ATOM | 3403 | O | LEU | B | 497 | 31.967 | 2.105 | 20.574 | 1.00 | 24.03 |
| | ATOM | 3404 | N | GLN | B | 498 | 33.798 | 0.797 | 20.447 | 1.00 | 26.17 |
| 60 | ATOM | 3405 | CA | GLN | B | 498 | 33.289 | -0.009 | 19.348 | 1.00 | 26.32 |
| | ATOM | 3406 | CB | GLN | B | 498 | 34.411 | -0.876 | 18.771 | 1.00 | 27.25 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3407 | CG | GLN | B | 498 | 33.967 | -1.796 | 17.645 | 1.00 | 32.67 |
| | ATOM | 3408 | CD | GLN | B | 498 | 34.965 | -2.912 | 17.374 | 1.00 | 38.39 |
| | ATOM | 3409 | OE1 | GLN | B | 498 | 35.737 | -3.298 | 18.254 | 1.00 | 36.78 |
| | ATOM | 3410 | NE2 | GLN | B | 498 | 34.953 | -3.437 | 16.153 | 1.00 | 33.18 |
| | ATOM | 3411 | C | GLN | B | 498 | 32.112 | -0.888 | 19.774 | 1.00 | 25.70 |
| 10 | ATOM | 3412 | O | GLN | B | 498 | 31.167 | -1.076 | 19.009 | 1.00 | 25.35 |
| | ATOM | 3413 | N | GLN | B | 499 | 32.173 | -1.434 | 20.986 | 1.00 | 24.01 |
| | ATOM | 3414 | CA | GLN | B | 499 | 31.093 | -2.281 | 21.487 | 1.00 | 25.34 |
| | ATOM | 3415 | CB | GLN | B | 499 | 31.501 | -2.935 | 22.815 | 1.00 | 28.38 |
| | ATOM | 3416 | CG | GLN | B | 499 | 32.537 | -4.056 | 22.669 | 1.00 | 29.13 |
| 15 | ATOM | 3417 | CD | GLN | B | 499 | 32.913 | -4.687 | 23.995 | 1.00 | 30.80 |
| | ATOM | 3418 | OE1 | GLN | B | 499 | 33.306 | -3.997 | 24.937 | 1.00 | 33.62 |
| | ATOM | 3419 | NE2 | GLN | B | 499 | 32.797 | -6.004 | 24.074 | 1.00 | 30.64 |
| | ATOM | 3420 | C | GLN | B | 499 | 29.842 | -1.430 | 21.693 | 1.00 | 25.70 |
| | ATOM | 3421 | O | GLN | B | 499 | 28.715 | -1.910 | 21.554 | 1.00 | 26.22 |
| 20 | ATOM | 3422 | N | GLN | B | 500 | 30.062 | -0.160 | 22.020 | 1.00 | 23.09 |
| | ATOM | 3423 | CA | GLN | B | 500 | 28.989 | 0.793 | 22.256 | 1.00 | 23.53 |
| | ATOM | 3424 | CB | GLN | B | 500 | 29.564 | 2.107 | 22.782 | 1.00 | 26.17 |
| | ATOM | 3425 | CG | GLN | B | 500 | 29.958 | 2.073 | 24.252 | 1.00 | 27.71 |
| | ATOM | 3426 | CD | GLN | B | 500 | 30.812 | 3.262 | 24.641 | 1.00 | 29.32 |
| 25 | ATOM | 3427 | OE1 | GLN | B | 500 | 30.559 | 4.386 | 24.207 | 1.00 | 28.48 |
| | ATOM | 3428 | NE2 | GLN | B | 500 | 31.831 | 3.021 | 25.463 | 1.00 | 25.07 |
| | ATOM | 3429 | C | GLN | B | 500 | 28.151 | 1.074 | 21.015 | 1.00 | 24.24 |
| | ATOM | 3430 | O | GLN | B | 500 | 26.923 | 0.949 | 21.053 | 1.00 | 24.40 |
| | ATOM | 3431 | N | HIS | B | 501 | 28.790 | 1.465 | 19.915 | 1.00 | 23.08 |
| 30 | ATOM | 3432 | CA | HIS | B | 501 | 28.004 | 1.739 | 18.724 | 1.00 | 26.92 |
| | ATOM | 3433 | CB | HIS | B | 501 | 28.791 | 2.577 | 17.697 | 1.00 | 32.00 |
| | ATOM | 3434 | CG | HIS | B | 501 | 29.988 | 1.896 | 17.105 | 1.00 | 36.97 |
| | ATOM | 3435 | CD2 | HIS | B | 501 | 30.122 | 0.710 | 16.465 | 1.00 | 40.32 |
| | ATOM | 3436 | ND1 | HIS | B | 501 | 31.224 | 2.505 | 17.042 | 1.00 | 37.88 |
| 35 | ATOM | 3437 | CE1 | HIS | B | 501 | 32.066 | 1.724 | 16.389 | 1.00 | 38.81 |
| | ATOM | 3438 | NE2 | HIS | B | 501 | 31.422 | 0.628 | 16.028 | 1.00 | 41.21 |
| | ATOM | 3439 | C | HIS | B | 501 | 27.451 | 0.457 | 18.123 | 1.00 | 25.91 |
| | ATOM | 3440 | O | HIS | B | 501 | 26.369 | 0.457 | 17.531 | 1.00 | 20.13 |
| | ATOM | 3441 | N | GLN | B | 502 | 28.165 | -0.648 | 18.317 | 1.00 | 24.94 |
| 40 | ATOM | 3442 | CA | GLN | B | 502 | 27.698 | -1.926 | 17.804 | 1.00 | 21.88 |
| | ATOM | 3443 | CB | GLN | B | 502 | 28.785 | -2.996 | 17.953 | 1.00 | 24.62 |
| | ATOM | 3444 | CG | GLN | B | 502 | 29.796 | -3.001 | 16.797 | 1.00 | 26.55 |
| | ATOM | 3445 | CD | GLN | B | 502 | 30.843 | -4.109 | 16.902 | 1.00 | 27.06 |
| | ATOM | 3446 | OE1 | GLN | B | 502 | 30.716 | -5.033 | 17.705 | 1.00 | 28.49 |
| 45 | ATOM | 3447 | NE2 | GLN | B | 502 | 31.882 | -4.018 | 16.078 | 1.00 | 21.90 |
| | ATOM | 3448 | C | GLN | B | 502 | 26.428 | -2.341 | 18.554 | 1.00 | 22.39 |
| | ATOM | 3449 | O | GLN | B | 502 | 25.464 | -2.807 | 17.944 | 1.00 | 22.24 |
| | ATOM | 3450 | N | ARG | B | 503 | 26.421 | -2.159 | 19.874 | 1.00 | 20.54 |
| | ATOM | 3451 | CA | ARG | B | 503 | 25.259 | -2.523 | 20.678 | 1.00 | 22.04 |
| 50 | ATOM | 3452 | CB | ARG | B | 503 | 25.602 | -2.519 | 22.180 | 1.00 | 22.51 |
| | ATOM | 3453 | CG | ARG | B | 503 | 24.451 | -3.022 | 23.077 | 1.00 | 23.34 |
| | ATOM | 3454 | CD | ARG | B | 503 | 24.853 | -3.110 | 24.550 | 1.00 | 22.18 |
| | ATOM | 3455 | NE | ARG | B | 503 | 23.743 | -3.546 | 25.395 | 1.00 | 19.62 |
| | ATOM | 3456 | CZ | ARG | B | 503 | 23.329 | -4.807 | 25.497 | 1.00 | 19.88 |
| 55 | ATOM | 3457 | NH1 | ARG | B | 503 | 23.933 | -5.765 | 24.809 | 1.00 | 16.40 |
| | ATOM | 3458 | NH2 | ARG | B | 503 | 22.303 | -5.110 | 26.280 | 1.00 | 19.71 |
| | ATOM | 3459 | C | ARG | B | 503 | 24.102 | -1.558 | 20.409 | 1.00 | 19.05 |
| | ATOM | 3460 | O | ARG | B | 503 | 22.945 | -1.968 | 20.351 | 1.00 | 18.87 |
| | ATOM | 3461 | N | LEU | B | 504 | 24.414 | -0.276 | 20.239 | 1.00 | 20.19 |
| 60 | ATOM | 3462 | CA | LEU | B | 504 | 23.375 | 0.714 | 19.969 | 1.00 | 19.33 |
| | ATOM | 3463 | CB | LEU | B | 504 | 23.972 | 2.117 | 19.855 | 1.00 | 16.25 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3464 | CG | LEU | B | 504 | 22.983 | 3.173 | 19.344 | 1.00 | 20.35 |
| | ATOM | 3465 | CD1 | LEU | B | 504 | 21.930 | 3.449 | 20.427 | 1.00 | 17.97 |
| | ATOM | 3466 | CD2 | LEU | B | 504 | 23.729 | 4.448 | 18.955 | 1.00 | 20.86 |
| | ATOM | 3467 | C | LEU | B | 504 | 22.659 | 0.357 | 18.667 | 1.00 | 21.22 |
| | ATOM | 3468 | O | LEU | B | 504 | 21.433 | 0.478 | 18.566 | 1.00 | 19.28 |
| 10 | ATOM | 3469 | N | ALA | B | 505 | 23.428 | -0.085 | 17.676 | 1.00 | 18.55 |
| | ATOM | 3470 | CA | ALA | B | 505 | 22.859 | -0.473 | 16.396 | 1.00 | 18.20 |
| | ATOM | 3471 | CB | ALA | B | 505 | 23.973 | -0.745 | 15.382 | 1.00 | 18.45 |
| | ATOM | 3472 | C | ALA | B | 505 | 21.986 | -1.716 | 16.562 | 1.00 | 19.54 |
| | ATOM | 3473 | O | ALA | B | 505 | 20.871 | -1.774 | 16.041 | 1.00 | 17.63 |
| 15 | ATOM | 3474 | N | GLN | B | 506 | 22.497 | -2.706 | 17.293 | 1.00 | 20.30 |
| | ATOM | 3475 | CA | GLN | B | 506 | 21.772 | -3.955 | 17.513 | 1.00 | 19.48 |
| | ATOM | 3476 | CB | GLN | B | 506 | 22.590 | -4.893 | 18.409 | 1.00 | 21.75 |
| | ATOM | 3477 | CG | GLN | B | 506 | 23.798 | -5.551 | 17.727 | 1.00 | 20.85 |
| | ATOM | 3478 | CD | GLN | B | 506 | 24.819 | -6.070 | 18.736 | 1.00 | 26.18 |
| 20 | ATOM | 3479 | OE1 | GLN | B | 506 | 24.564 | -6.084 | 19.943 | 1.00 | 21.83 |
| | ATOM | 3480 | NE2 | GLN | B | 506 | 25.977 | -6.499 | 18.245 | 1.00 | 25.39 |
| | ATOM | 3481 | C | GLN | B | 506 | 20.421 | -3.672 | 18.166 | 1.00 | 21.39 |
| | ATOM | 3482 | O | GLN | B | 506 | 19.396 | -4.233 | 17.766 | 1.00 | 20.87 |
| | ATOM | 3483 | N | LEU | B | 507 | 20.433 | -2.800 | 19.171 | 1.00 | 19.52 |
| 25 | ATOM | 3484 | CA | LEU | B | 507 | 19.219 | -2.418 | 19.884 | 1.00 | 23.04 |
| | ATOM | 3485 | CB | LEU | B | 507 | 19.548 | -1.455 | 21.030 | 1.00 | 22.82 |
| | ATOM | 3486 | CG | LEU | B | 507 | 20.182 | -2.011 | 22.313 | 1.00 | 26.12 |
| | ATOM | 3487 | CD1 | LEU | B | 507 | 20.203 | -0.916 | 23.360 | 1.00 | 29.33 |
| | ATOM | 3488 | CD2 | LEU | B | 507 | 19.415 | -3.213 | 22.816 | 1.00 | 27.80 |
| 30 | ATOM | 3489 | C | LEU | B | 507 | 18.212 | -1.730 | 18.971 | 1.00 | 22.19 |
| | ATOM | 3490 | Q | LEU | B | 507 | 17.036 | -2.070 | 18.964 | 1.00 | 23.00 |
| | ATOM | 3491 | N | LEU | B | 508 | 18.678 | -0.745 | 18.214 | 1.00 | 21.53 |
| | ATOM | 3492 | CA | LEU | B | 508 | 17.797 | 0.006 | 17.332 | 1.00 | 20.60 |
| | ATOM | 3493 | CB | LEU | B | 508 | 18.535 | 1.236 | 16.805 | 1.00 | 17.57 |
| 35 | ATOM | 3494 | CG | LEU | B | 508 | 18.934 | 2.218 | 17.913 | 1.00 | 17.67 |
| | ATOM | 3495 | CD1 | LEU | B | 508 | 19.566 | 3.446 | 17.301 | 1.00 | 20.04 |
| | ATOM | 3496 | CD2 | LEU | B | 508 | 17.724 | 2.611 | 18.725 | 1.00 | 18.49 |
| | ATOM | 3497 | C | LEU | B | 508 | 17.235 | -0.831 | 16.183 | 1.00 | 21.17 |
| | ATOM | 3498 | O | LEU | B | 508 | 16.118 | -0.597 | 15.728 | 1.00 | 21.88 |
| 40 | ATOM | 3499 | N | LEU | B | 509 | 18.000 | -1.813 | 15.713 | 1.00 | 21.89 |
| | ATOM | 3500 | CA | LEU | B | 509 | 17.511 | -2.657 | 14.631 | 1.00 | 22.81 |
| | ATOM | 3501 | CB | LEU | B | 509 | 18.603 | -3.597 | 14.145 | 1.00 | 22.65 |
| | ATOM | 3502 | CG | LEU | B | 509 | 19.645 | -2.891 | 13.278 | 1.00 | 29.11 |
| | ATOM | 3503 | CD1 | LEU | B | 509 | 20.697 | -3.888 | 12.829 | 1.00 | 25.69 |
| 45 | ATOM | 3504 | CD2 | LEU | B | 509 | 18.965 | -2.248 | 12.082 | 1.00 | 27.92 |
| | ATOM | 3505 | C | LEU | B | 509 | 16.302 | -3.462 | 15.095 | 1.00 | 23.32 |
| | ATOM | 3506 | O | LEU | B | 509 | 15.409 | -3.759 | 14.303 | 1.00 | 23.36 |
| | ATOM | 3507 | N | ILE | B | 510 | 16.264 | -3.796 | 16.380 | 1.00 | 23.36 |
| | ATOM | 3508 | CA | ILE | B | 510 | 15.148 | -4.562 | 16.912 | 1.00 | 20.99 |
| 50 | ATOM | 3509 | CB | ILE | B | 510 | 15.448 | -5.041 | 18.361 | 1.00 | 28.60 |
| | ATOM | 3510 | CG2 | ILE | B | 510 | 14.162 | -5.435 | 19.075 | 1.00 | 28.10 |
| | ATOM | 3511 | CG1 | ILE | B | 510 | 16.383 | -6.260 | 18.308 | 1.00 | 26.57 |
| | ATOM | 3512 | CD1 | ILE | B | 510 | 17.429 | -6.301 | 19.419 | 1.00 | 30.14 |
| | ATOM | 3513 | C | ILE | B | 510 | 13.852 | -3.746 | 16.846 | 1.00 | 17.65 |
| 55 | ATOM | 3514 | O | ILE | B | 510 | 12.767 | -4.308 | 16.759 | 1.00 | 16.11 |
| | ATOM | 3515 | N | LEU | B | 511 | 13.961 | -2.421 | 16.867 | 1.00 | 18.12 |
| | ATOM | 3516 | CA | LEU | B | 511 | 12.772 | -1.574 | 16.774 | 1.00 | 16.95 |
| | ATOM | 3517 | CB | LEU | B | 511 | 13.147 | -0.100 | 16.981 | 1.00 | 22.66 |
| | ATOM | 3518 | CG | LEU | B | 511 | 13.607 | 0.262 | 18.406 | 1.00 | 22.13 |
| 60 | ATOM | 3519 | CD1 | LEU | B | 511 | 13.404 | 1.751 | 18.652 | 1.00 | 25.29 |
| | ATOM | 3520 | CD2 | LEU | B | 511 | 12.830 | -0.549 | 19.425 | 1.00 | 25.08 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 3521 | C | LEU | B | 511 | 12.112 | -1.771 | 15.397 | 1.00 | 16.65 |
| | ATOM | 3522 | O | LEU | B | 511 | 10.915 | -1.578 | 15.242 | 1.00 | 17.09 |
| | ATOM | 3523 | N | SER | B | 512 | 12.901 | -2.161 | 14.401 | 1.00 | 15.83 |
| | ATOM | 3524 | CA | SER | B | 512 | 12.355 | -2.408 | 13.072 | 1.00 | 18.66 |
| | ATOM | 3525 | CB | SER | B | 512 | 13.484 | -2.644 | 12.074 | 1.00 | 17.62 |
| 10 | ATOM | 3526 | OG | SER | B | 512 | 13.079 | -3.550 | 11.062 | 1.00 | 32.77 |
| | ATOM | 3527 | C | SER | B | 512 | 11.454 | -3.638 | 13.154 | 1.00 | 18.54 |
| | ATOM | 3528 | O | SER | B | 512 | 10.373 | -3.683 | 12.545 | 1.00 | 17.01 |
| | ATOM | 3529 | N | HIS | B | 513 | 11.899 | -4.625 | 13.929 | 1.00 | 15.54 |
| | ATOM | 3530 | CA | HIS | B | 513 | 11.141 | -5.860 | 14.115 | 1.00 | 17.67 |
| 15 | ATOM | 3531 | CB | HIS | B | 513 | 12.013 | -6.916 | 14.790 | 1.00 | 19.03 |
| | ATOM | 3532 | CG | HIS | B | 513 | 13.063 | -7.475 | 13.886 | 1.00 | 27.06 |
| | ATOM | 3533 | CD2 | HIS | B | 513 | 12.980 | -8.364 | 12.868 | 1.00 | 28.40 |
| | ATOM | 3534 | ND1 | HIS | B | 513 | 14.378 | -7.066 | 13.932 | 1.00 | 28.92 |
| | ATOM | 3535 | CE1 | HIS | B | 513 | 15.061 | -7.678 | 12.981 | 1.00 | 30.75 |
| 20 | ATOM | 3536 | NE2 | HIS | B | 513 | 14.235 | -8.472 | 12.321 | 1.00 | 30.08 |
| | ATOM | 3537 | C | HIS | B | 513 | 9.895 | -5.602 | 14.958 | 1.00 | 15.35 |
| | ATOM | 3538 | O | HIS | B | 513 | 8.846 | -6.192 | 14.704 | 1.00 | 14.83 |
| | ATOM | 3539 | N | ILE | B | 514 | 10.012 | -4.744 | 15.942 | 1.00 | 13.35 |
| | ATOM | 3540 | CA | ILE | B | 514 | 8.865 | -4.417 | 16.776 | 1.00 | 15.48 |
| 25 | ATOM | 3541 | CB | ILE | B | 514 | 9.295 | -3.534 | 17.967 | 1.00 | 20.02 |
| | ATOM | 3542 | CG2 | ILE | B | 514 | 8.067 | -2.918 | 18.650 | 1.00 | 12.84 |
| | ATOM | 3543 | CG1 | ILE | B | 514 | 10.093 | -4.397 | 18.962 | 1.00 | 22.87 |
| | ATOM | 3544 | CD1 | ILE | B | 514 | 10.691 | -3.641 | 20.115 | 1.00 | 29.62 |
| | ATOM | 3545 | C | ILE | B | 514 | 7.797 | -3.717 | 15.923 | 1.00 | 15.16 |
| 30 | ATOM | 3546 | O | ILE | B | 514 | 6.606 | -3.972 | 16.078 | 1.00 | 16.61 |
| | ATOM | 3547 | N | ARG | B | 515 | 8.224 | -2.823 | 15.030 | 1.00 | 16.33 |
| | ATOM | 3548 | CA | ARG | B | 515 | 7.280 | -2.138 | 14.150 | 1.00 | 17.54 |
| | ATOM | 3549 | CB | ARG | B | 515 | 8.010 | -1.173 | 13.214 | 1.00 | 20.15 |
| | ATOM | 3550 | CG | ARG | B | 515 | 7.080 | -0.454 | 12.234 | 1.00 | 21.47 |
| 35 | ATOM | 3551 | CD | ARG | B | 515 | 6.407 | 0.749 | 12.891 | 1.00 | 26.05 |
| | ATOM | 3552 | NE | ARG | B | 515 | 7.220 | 1.948 | 12.716 | 1.00 | 24.91 |
| | ATOM | 3553 | CZ | ARG | B | 515 | 6.734 | 3.175 | 12.547 | 1.00 | 24.61 |
| | ATOM | 3554 | NH1 | ARG | B | 515 | 5.424 | 3.393 | 12.522 | 1.00 | 22.46 |
| | ATOM | 3555 | NH2 | ARG | B | 515 | 7.569 | 4.182 | 12.374 | 1.00 | 23.15 |
| 40 | ATOM | 3556 | C | ARG | B | 515 | 6.545 | -3.182 | 13.304 | 1.00 | 16.60 |
| | ATOM | 3557 | O | ARG | B | 515 | 5.332 | -3.093 | 13.087 | 1.00 | 14.51 |
| | ATOM | 3558 | N | HIS | B | 516 | 7.298 | -4.171 | 12.827 | 1.00 | 18.50 |
| | ATOM | 3559 | CA | HIS | B | 516 | 6.743 | -5.237 | 11.997 | 1.00 | 17.26 |
| | ATOM | 3560 | CB | HIS | B | 516 | 7.861 | -6.176 | 11.533 | 1.00 | 18.14 |
| 45 | ATOM | 3561 | CG | HIS | B | 516 | 7.405 | -7.223 | 10.568 | 1.00 | 24.87 |
| | ATOM | 3562 | CD2 | HIS | B | 516 | 7.060 | -8.521 | 10.754 | 1.00 | 26.64 |
| | ATOM | 3563 | ND1 | HIS | B | 516 | 7.258 | -6.978 | 9.220 | 1.00 | 21.82 |
| | ATOM | 3564 | CE1 | HIS | B | 516 | 6.839 | -8.078 | 8.619 | 1.00 | 28.42 |
| | ATOM | 3565 | NE2 | HIS | B | 516 | 6.711 | -9.028 | 9.526 | 1.00 | 24.47 |
| 50 | ATOM | 3566 | C | HIS | B | 516 | 5.685 | -6.028 | 12.759 | 1.00 | 16.87 |
| | ATOM | 3567 | O | HIS | B | 516 | 4.596 | -6.303 | 12.240 | 1.00 | 14.81 |
| | ATOM | 3568 | N | MET | B | 517 | 5.999 | -6.396 | 13.997 | 1.00 | 16.48 |
| | ATOM | 3569 | CA | MET | B | 517 | 5.049 | -7.162 | 14.801 | 1.00 | 15.39 |
| | ATOM | 3570 | CB | MET | B | 517 | 5.701 | -7.587 | 16.114 | 1.00 | 21.05 |
| 55 | ATOM | 3571 | CG | MET | B | 517 | 6.790 | -8.638 | 15.917 | 1.00 | 20.76 |
| | ATOM | 3572 | SD | MET | B | 517 | 7.380 | -9.320 | 17.470 | 1.00 | 23.96 |
| | ATOM | 3573 | CE | MET | B | 517 | 8.104 | -7.879 | 18.226 | 1.00 | 20.45 |
| | ATOM | 3574 | C | MET | B | 517 | 3.789 | -6.368 | 15.080 | 1.00 | 16.23 |
| | ATOM | 3575 | O | MET | B | 517 | 2.688 | -6.924 | 15.148 | 1.00 | 16.02 |
| 60 | ATOM | 3576 | N | SER | B | 518 | 3.954 | -5.060 | 15.247 | 1.00 | 13.32 |
| | ATOM | 3577 | CA | SER | B | 518 | 2.827 | -4.186 | 15.505 | 1.00 | 16.34 |

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 3578 | CB | SER | B | 518 | 3.316 | -2.765 | 15.835 | 1.00 | 17.48 |
| | ATOM | 3579 | OG | SER | B | 518 | 2.234 | -1.840 | 15.843 | 1.00 | 17.46 |
| | ATOM | 3580 | C | SER | B | 518 | 1.906 | -4.147 | 14.284 | 1.00 | 14.73 |
| | ATOM | 3581 | O | SER | B | 518 | 0.688 | -4.247 | 14.417 | 1.00 | 19.16 |
| | ATOM | 3582 | N | ASN | B | 519 | 2.474 | -4.006 | 13.091 | 1.00 | 14.52 |
| 10 | ATOM | 3583 | CA | ASN | B | 519 | 1.622 | -3.953 | 11.907 | 1.00 | 15.35 |
| | ATOM | 3584 | CB | ASN | B | 519 | 2.432 | -3.509 | 10.698 | 1.00 | 19.21 |
| | ATOM | 3585 | CG | ASN | B | 519 | 2.700 | -2.029 | 10.729 | 1.00 | 20.58 |
| | ATOM | 3586 | OD1 | ASN | B | 519 | 1.839 | -1.258 | 11.150 | 1.00 | 26.36 |
| | ATOM | 3587 | ND2 | ASN | B | 519 | 3.891 | -1.618 | 10.307 | 1.00 | 19.62 |
| 15 | ATOM | 3588 | C | ASN | B | 519 | 0.911 | -5.280 | 11.658 | 1.00 | 16.74 |
| | ATOM | 3589 | O | ASN | B | 519 | -0.265 | -5.299 | 11.297 | 1.00 | 20.58 |
| | ATOM | 3590 | N | LYS | B | 520 | 1.608 | -6.387 | 11.885 | 1.00 | 18.60 |
| | ATOM | 3591 | CA | LYS | B | 520 | 0.992 | -7.699 | 11.717 | 1.00 | 20.04 |
| | ATOM | 3592 | CB | LYS | B | 520 | 2.038 | -8.801 | 11.872 | 1.00 | 25.44 |
| 20 | ATOM | 3593 | CG | LYS | B | 520 | 3.037 | -8.849 | 10.728 | 1.00 | 31.68 |
| | ATOM | 3594 | CD | LYS | B | 520 | 2.507 | -9.663 | 9.558 | 1.00 | 42.56 |
| | ATOM | 3595 | CE | LYS | B | 520 | 2.186 | -8.778 | 8.364 | 1.00 | 45.61 |
| | ATOM | 3596 | NZ | LYS | B | 520 | 1.435 | -9.526 | 7.312 | 1.00 | 46.00 |
| | ATOM | 3597 | C | LYS | B | 520 | -0.099 | -7.868 | 12.769 | 1.00 | 18.88 |
| 25 | ATOM | 3598 | O | LYS | B | 520 | -1.183 | -8.358 | 12.478 | 1.00 | 21.75 |
| | ATOM | 3599 | N | GLY | B | 521 | 0.191 | -7.455 | 13.998 | 1.00 | 17.83 |
| | ATOM | 3600 | CA | GLY | B | 521 | -0.792 | -7.569 | 15.058 | 1.00 | 16.19 |
| | ATOM | 3601 | C | GLY | B | 521 | -2.000 | -6.674 | 14.833 | 1.00 | 16.59 |
| | ATOM | 3602 | O | GLY | B | 521 | -3.128 | -7.060 | 15.125 | 1.00 | 16.57 |
| 30 | ATOM | 3603 | N | MET | B | 522 | -1.766 | -5.467 | 14.326 | 1.00 | 17.48 |
| | ATOM | 3604 | CA | MET | B | 522 | -2.852 | -4.527 | 14.042 | 1.00 | 18.25 |
| | ATOM | 3605 | CB | MET | B | 522 | -2.276 | -3.212 | 13.516 | 1.00 | 21.27 |
| | ATOM | 3606 | CG | MET | B | 522 | -3.190 | -2.018 | 13.707 | 1.00 | 26.97 |
| | ATOM | 3607 | SD | MET | B | 522 | -3.199 | -1.477 | 15.417 | 1.00 | 30.35 |
| 35 | ATOM | 3608 | CE | MET | B | 522 | -1.659 | -0.605 | 15.475 | 1.00 | 29.86 |
| | ATOM | 3609 | C | MET | B | 522 | -3.794 | -5.119 | 12.989 | 1.00 | 18.68 |
| | ATOM | 3610 | O | MET | B | 522 | -5.022 | -5.008 | 13.097 | 1.00 | 18.80 |
| | ATOM | 3611 | N | GLU | B | 523 | -3.205 | -5.731 | 11.966 | 1.00 | 18.22 |
| | ATOM | 3612 | CA | GLU | B | 523 | -3.968 | -6.357 | 10.889 | 1.00 | 23.41 |
| 40 | ATOM | 3613 | CB | GLU | B | 523 | -3.031 | -6.946 | 9.830 | 1.00 | 28.74 |
| | ATOM | 3614 | CG | GLU | B | 523 | -2.224 | -5.935 | 9.030 | 1.00 | 34.42 |
| | ATOM | 3615 | CD | GLU | B | 523 | -1.095 | -6.597 | 8.239 | 1.00 | 45.58 |
| | ATOM | 3616 | OE1 | GLU | B | 523 | -0.131 | -5.894 | 7.857 | 1.00 | 49.48 |
| | ATOM | 3617 | OE2 | GLU | B | 523 | -1.169 | -7.825 | 7.999 | 1.00 | 45.97 |
| 45 | ATOM | 3618 | C | GLU | B | 523 | -4.812 | -7.482 | 11.465 | 1.00 | 23.98 |
| | ATOM | 3619 | O | GLU | B | 523 | -5.993 | -7.616 | 11.147 | 1.00 | 22.08 |
| | ATOM | 3620 | N | HIS | B | 524 | -4.187 | -8.287 | 12.326 | 1.00 | 23.46 |
| | ATOM | 3621 | CA | HIS | B | 524 | -4.846 | -9.428 | 12.952 | 1.00 | 26.20 |
| | ATOM | 3622 | CB | HIS | B | 524 | -3.824 | -10.245 | 13.743 | 1.00 | 27.26 |
| 50 | ATOM | 3623 | CG | HIS | B | 524 | -4.378 | -11.509 | 14.321 | 1.00 | 30.91 |
| | ATOM | 3624 | CD2 | HIS | B | 524 | -4.308 | -12.792 | 13.892 | 1.00 | 30.90 |
| | ATOM | 3625 | ND1 | HIS | B | 524 | -5.107 | -11.537 | 15.490 | 1.00 | 28.87 |
| | ATOM | 3626 | CE1 | HIS | B | 524 | -5.461 | -12.780 | 15.757 | 1.00 | 30.45 |
| | ATOM | 3627 | NE2 | HIS | B | 524 | -4.989 | -13.561 | 14.803 | 1.00 | 29.19 |
| 55 | ATOM | 3628 | C | HIS | B | 524 | -5.996 | -9.025 | 13.870 | 1.00 | 27.69 |
| | ATOM | 3629 | O | HIS | B | 524 | -7.061 | -9.656 | 13.860 | 1.00 | 25.00 |
| | ATOM | 3630 | N | LEU | B | 525 | -5.777 | -7.977 | 14.655 | 1.00 | 23.84 |
| | ATOM | 3631 | CA | LEU | B | 525 | -6.786 | -7.492 | 15.588 | 1.00 | 25.77 |
| | ATOM | 3632 | CB | LEU | B | 525 | -6.217 | -6.358 | 16.444 | 1.00 | 22.22 |
| 60 | ATOM | 3633 | CG | LEU | B | 525 | -7.164 | -5.778 | 17.498 | 1.00 | 26.81 |
| | ATOM | 3634 | CD1 | LEU | B | 525 | -7.763 | -6.922 | 18.321 | 1.00 | 23.32 |

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|----|------|------|-----|-----|---|-----|---------|---------|--------|------|-------|
| 5 | ATOM | 3635 | CD2 | LEU | B | 525 | -6.414 | -4.793 | 18.399 | 1.00 | 18.95 |
| | ATOM | 3636 | C | LEU | B | 525 | -8.013 | -6.995 | 14.842 | 1.00 | 26.84 |
| | ATOM | 3637 | O | LEU | B | 525 | -9.154 | -7.247 | 15.249 | 1.00 | 26.73 |
| | ATOM | 3638 | N | TYR | B | 526 | -7.764 | -6.271 | 13.757 | 1.00 | 26.86 |
| | ATOM | 3639 | CA | TYR | B | 526 | -8.819 | -5.726 | 12.918 | 1.00 | 30.89 |
| 10 | ATOM | 3640 | CB | TYR | B | 526 | -8.201 | -4.818 | 11.854 | 1.00 | 34.31 |
| | ATOM | 3641 | CG | TYR | B | 526 | -9.183 | -4.223 | 10.878 | 1.00 | 43.50 |
| | ATOM | 3642 | CD1 | TYR | B | 526 | -10.058 | -3.211 | 11.267 | 1.00 | 47.66 |
| | ATOM | 3643 | CE1 | TYR | B | 526 | -10.943 | -2.636 | 10.357 | 1.00 | 48.85 |
| | ATOM | 3644 | CD2 | TYR | B | 526 | -9.218 | -4.651 | 9.552 | 1.00 | 48.52 |
| 15 | ATOM | 3645 | CE2 | TYR | B | 526 | -10.098 | -4.083 | 8.634 | 1.00 | 52.43 |
| | ATOM | 3646 | CZ | TYR | B | 526 | -10.955 | -3.077 | 9.043 | 1.00 | 51.67 |
| | ATOM | 3647 | OH | TYR | B | 526 | -11.810 | -2.504 | 8.129 | 1.00 | 57.01 |
| | ATOM | 3648 | C | TYR | B | 526 | -9.577 | -6.880 | 12.265 | 1.00 | 30.90 |
| | ATOM | 3649 | O | TYR | B | 526 | -10.793 | -6.829 | 12.113 | 1.00 | 31.48 |
| 20 | ATOM | 3650 | N | SER | B | 527 | -8.849 | -7.926 | 11.889 | 1.00 | 31.39 |
| | ATOM | 3651 | CA | SER | B | 527 | -9.460 | -9.095 | 11.266 | 1.00 | 33.73 |
| | ATOM | 3652 | CB | SER | B | 527 | -8.377 | -10.048 | 10.749 | 1.00 | 34.13 |
| | ATOM | 3653 | OG | SER | B | 527 | -8.945 | -11.222 | 10.196 | 1.00 | 43.67 |
| | ATOM | 3654 | C | SER | B | 527 | -10.339 | -9.813 | 12.288 | 1.00 | 34.34 |
| 25 | ATOM | 3655 | O | SER | B | 527 | -11.446 | -10.261 | 11.973 | 1.00 | 33.42 |
| | ATOM | 3656 | N | MET | B | 528 | -9.840 | -9.916 | 13.517 | 1.00 | 31.66 |
| | ATOM | 3657 | CA | MET | B | 528 | -10.574 | -10.572 | 14.589 | 1.00 | 29.77 |
| | ATOM | 3658 | CB | MET | B | 528 | -9.682 | -10.743 | 15.820 | 1.00 | 32.96 |
| | ATOM | 3659 | CG | MET | B | 528 | -8.651 | -11.859 | 15.699 | 1.00 | 33.47 |
| 30 | ATOM | 3660 | SD | MET | B | 528 | -9.359 | -13.427 | 15.134 | 1.00 | 38.28 |
| | ATOM | 3661 | CE | MET | B | 528 | -10.265 | -13.915 | 16.579 | 1.00 | 36.01 |
| | ATOM | 3662 | C | MET | B | 528 | -11.800 | -9.747 | 14.953 | 1.00 | 29.42 |
| | ATOM | 3663 | O | MET | B | 528 | -12.835 | -10.293 | 15.331 | 1.00 | 28.65 |
| | ATOM | 3664 | N | LYS | B | 529 | -11.673 | -8.429 | 14.850 | 1.00 | 30.64 |
| 35 | ATOM | 3665 | CA | LYS | B | 529 | -12.781 | -7.533 | 15.149 | 1.00 | 31.80 |
| | ATOM | 3666 | CB | LYS | B | 529 | -12.323 | -6.079 | 15.027 | 1.00 | 32.86 |
| | ATOM | 3667 | CG | LYS | B | 529 | -13.436 | -5.043 | 15.114 | 1.00 | 36.42 |
| | ATOM | 3668 | CD | LYS | B | 529 | -13.114 | -3.852 | 14.224 | 1.00 | 41.74 |
| | ATOM | 3669 | CE | LYS | B | 529 | -13.734 | -2.564 | 14.741 | 1.00 | 43.45 |
| 40 | ATOM | 3670 | NZ | LYS | B | 529 | -15.221 | -2.569 | 14.634 | 1.00 | 46.51 |
| | ATOM | 3671 | C | LYS | B | 529 | -13.857 | -7.840 | 14.116 | 1.00 | 36.60 |
| | ATOM | 3672 | O | LYS | B | 529 | -15.049 | -7.877 | 14.424 | 1.00 | 34.04 |
| | ATOM | 3673 | N | CYS | B | 530 | -13.407 | -8.083 | 12.889 | 1.00 | 40.04 |
| | ATOM | 3674 | CA | CYS | B | 530 | -14.286 | -8.409 | 11.773 | 1.00 | 44.58 |
| 45 | ATOM | 3675 | CB | CYS | B | 530 | -13.460 | -8.535 | 10.491 | 1.00 | 50.64 |
| | ATOM | 3676 | SG | CYS | B | 530 | -13.369 | -7.034 | 9.504 | 1.00 | 67.65 |
| | ATOM | 3677 | C | CYS | B | 530 | -15.065 | -9.692 | 12.016 | 1.00 | 42.88 |
| | ATOM | 3678 | O | CYS | B | 530 | -16.274 | -9.741 | 11.807 | 1.00 | 40.15 |
| | ATOM | 3679 | N | LYS | B | 531 | -14.360 | -10.733 | 12.447 | 1.00 | 41.92 |
| 50 | ATOM | 3680 | CA | LYS | B | 531 | -14.980 | -12.023 | 12.728 | 1.00 | 42.60 |
| | ATOM | 3681 | CB | LYS | B | 531 | -13.907 | -13.091 | 12.927 | 1.00 | 44.77 |
| | ATOM | 3682 | C | LYS | B | 531 | -15.844 | -11.907 | 13.977 | 1.00 | 44.43 |
| | ATOM | 3683 | O | LYS | B | 531 | -16.623 | -12.804 | 14.296 | 1.00 | 44.09 |
| | ATOM | 3684 | N | ASN | B | 532 | -15.678 | -10.793 | 14.685 | 1.00 | 44.98 |
| 55 | ATOM | 3685 | CA | ASN | B | 532 | -16.437 | -10.496 | 15.893 | 1.00 | 44.10 |
| | ATOM | 3686 | CB | ASN | B | 532 | -17.833 | -10.003 | 15.506 | 1.00 | 45.14 |
| | ATOM | 3687 | CG | ASN | B | 532 | -18.526 | -9.271 | 16.633 | 1.00 | 46.54 |
| | ATOM | 3688 | OD1 | ASN | B | 532 | -19.729 | -9.424 | 16.837 | 1.00 | 50.62 |
| | ATOM | 3689 | ND2 | ASN | B | 532 | -17.771 | -8.471 | 17.375 | 1.00 | 46.07 |
| 60 | ATOM | 3690 | C | ASN | B | 532 | -16.557 | -11.657 | 16.882 | 1.00 | 43.34 |
| | ATOM | 3691 | O | ASN | B | 532 | -17.655 | -11.994 | 17.321 | 1.00 | 41.42 |

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|----|------|------|-----|-----|---|-----|---------|---------|--------|------|-------|
| 5 | ATOM | 3692 | N | VAL | B | 533 | -15.434 | -12.264 | 17.243 | 1.00 | 43.45 |
| | ATOM | 3693 | CA | VAL | B | 533 | -15.471 | -13.371 | 18.190 | 1.00 | 44.06 |
| | ATOM | 3694 | CB | VAL | B | 533 | -14.170 | -14.219 | 18.120 | 1.00 | 45.56 |
| | ATOM | 3695 | CG1 | VAL | B | 533 | -13.661 | -14.263 | 16.683 | 1.00 | 45.67 |
| | ATOM | 3696 | CG2 | VAL | B | 533 | -13.107 | -13.644 | 19.045 | 1.00 | 44.16 |
| 10 | ATOM | 3697 | C | VAL | B | 533 | -15.670 | -12.835 | 19.611 | 1.00 | 43.24 |
| | ATOM | 3698 | O | VAL | B | 533 | -15.894 | -13.602 | 20.548 | 1.00 | 44.21 |
| | ATOM | 3699 | N | VAL | B | 534 | -15.596 | -11.511 | 19.755 | 1.00 | 40.44 |
| | ATOM | 3700 | CA | VAL | B | 534 | -15.765 | -10.849 | 21.049 | 1.00 | 37.80 |
| | ATOM | 3701 | CB | VAL | B | 534 | -14.630 | -11.259 | 22.038 | 1.00 | 36.38 |
| 15 | ATOM | 3702 | CG1 | VAL | B | 534 | -13.324 | -10.575 | 21.658 | 1.00 | 34.35 |
| | ATOM | 3703 | CG2 | VAL | B | 534 | -15.021 | -10.910 | 23.463 | 1.00 | 39.34 |
| | ATOM | 3704 | C | VAL | B | 534 | -15.752 | -9.329 | 20.857 | 1.00 | 37.97 |
| | ATOM | 3705 | O | VAL | B | 534 | -15.026 | -8.808 | 20.008 | 1.00 | 39.45 |
| | ATOM | 3706 | N | PRO | B | 535 | -16.575 | -8.597 | 21.625 | 1.00 | 37.81 |
| 20 | ATOM | 3707 | CD | PRO | B | 535 | -17.529 | -9.078 | 22.640 | 1.00 | 38.74 |
| | ATOM | 3708 | CA | PRO | B | 535 | -16.608 | -7.135 | 21.492 | 1.00 | 36.79 |
| | ATOM | 3709 | CB | PRO | B | 535 | -17.846 | -6.729 | 22.288 | 1.00 | 36.98 |
| | ATOM | 3710 | CG | PRO | B | 535 | -18.004 | -7.809 | 23.298 | 1.00 | 39.77 |
| | ATOM | 3711 | C | PRO | B | 535 | -15.338 | -6.494 | 22.049 | 1.00 | 33.95 |
| 25 | ATOM | 3712 | O | PRO | B | 535 | -14.786 | -6.963 | 23.040 | 1.00 | 34.93 |
| | ATOM | 3713 | N | LEU | B | 536 | -14.881 | -5.426 | 21.409 | 1.00 | 33.42 |
| | ATOM | 3714 | CA | LEU | B | 536 | -13.675 | -4.732 | 21.851 | 1.00 | 33.40 |
| | ATOM | 3715 | CB | LEU | B | 536 | -12.829 | -4.314 | 20.647 | 1.00 | 29.31 |
| | ATOM | 3716 | CG | LEU | B | 536 | -12.219 | -5.433 | 19.798 | 1.00 | 30.06 |
| 30 | ATOM | 3717 | CD1 | LEU | B | 536 | -11.344 | -4.822 | 18.714 | 1.00 | 30.85 |
| | ATOM | 3718 | CD2 | LEU | B | 536 | -11.398 | -6.370 | 20.676 | 1.00 | 28.96 |
| | ATOM | 3719 | C | LEU | B | 536 | -14.036 | -3.498 | 22.666 | 1.00 | 30.50 |
| | ATOM | 3720 | O | LEU | B | 536 | -15.024 | -2.829 | 22.383 | 1.00 | 29.91 |
| | ATOM | 3721 | N | TYR | B | 537 | -13.231 | -3.194 | 23.676 | 1.00 | 28.69 |
| 35 | ATOM | 3722 | CA | TYR | B | 537 | -13.494 | -2.032 | 24.505 | 1.00 | 29.89 |
| | ATOM | 3723 | CB | TYR | B | 537 | -12.618 | -2.071 | 25.750 | 1.00 | 32.50 |
| | ATOM | 3724 | CG | TYR | B | 537 | -12.849 | -3.327 | 26.543 | 1.00 | 39.46 |
| | ATOM | 3725 | CD1 | TYR | B | 537 | -13.923 | -3.431 | 27.421 | 1.00 | 41.90 |
| | ATOM | 3726 | CE1 | TYR | B | 537 | -14.174 | -4.609 | 28.118 | 1.00 | 45.72 |
| 40 | ATOM | 3727 | CD2 | TYR | B | 537 | -12.022 | -4.435 | 26.379 | 1.00 | 47.39 |
| | ATOM | 3728 | CE2 | TYR | B | 537 | -12.262 | -5.620 | 27.072 | 1.00 | 49.93 |
| | ATOM | 3729 | CZ | TYR | B | 537 | -13.340 | -5.699 | 27.940 | 1.00 | 48.80 |
| | ATOM | 3730 | OH | TYR | B | 537 | -13.582 | -6.872 | 28.624 | 1.00 | 53.90 |
| | ATOM | 3731 | C | TYR | B | 537 | -13.262 | -0.761 | 23.709 | 1.00 | 27.09 |
| 45 | ATOM | 3732 | O | TYR | B | 537 | -12.518 | -0.757 | 22.729 | 1.00 | 26.15 |
| | ATOM | 3733 | N | ASP | B | 538 | -13.909 | 0.315 | 24.141 | 1.00 | 26.12 |
| | ATOM | 3734 | CA | ASP | B | 538 | -13.830 | 1.598 | 23.461 | 1.00 | 25.27 |
| | ATOM | 3735 | CB | ASP | B | 538 | -14.748 | 2.598 | 24.164 | 1.00 | 28.85 |
| | ATOM | 3736 | CG | ASP | B | 538 | -16.227 | 2.285 | 23.940 | 1.00 | 33.90 |
| 50 | ATOM | 3737 | OD1 | ASP | B | 538 | -17.052 | 2.613 | 24.819 | 1.00 | 32.68 |
| | ATOM | 3738 | OD2 | ASP | B | 538 | -16.562 | 1.707 | 22.882 | 1.00 | 38.26 |
| | ATOM | 3739 | C | ASP | B | 538 | -12.447 | 2.217 | 23.261 | 1.00 | 25.18 |
| | ATOM | 3740 | O | ASP | B | 538 | -12.120 | 2.626 | 22.147 | 1.00 | 26.41 |
| | ATOM | 3741 | N | LEU | B | 539 | -11.637 | 2.309 | 24.313 | 1.00 | 20.76 |
| 55 | ATOM | 3742 | CA | LEU | B | 539 | -10.312 | 2.911 | 24.150 | 1.00 | 19.65 |
| | ATOM | 3743 | CB | LEU | B | 539 | -9.567 | 2.991 | 25.496 | 1.00 | 17.48 |
| | ATOM | 3744 | CG | LEU | B | 539 | -8.116 | 3.511 | 25.469 | 1.00 | 16.46 |
| | ATOM | 3745 | CD1 | LEU | B | 539 | -8.051 | 4.892 | 24.838 | 1.00 | 16.43 |
| | ATOM | 3746 | CD2 | LEU | B | 539 | -7.564 | 3.569 | 26.895 | 1.00 | 15.57 |
| 60 | ATOM | 3747 | C | LEU | B | 539 | -9.484 | 2.127 | 23.127 | 1.00 | 16.75 |
| | ATOM | 3748 | O | LEU | B | 539 | -8.862 | 2.716 | 22.249 | 1.00 | 20.36 |

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|----|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|
| 5 | ATOM | 3749 | N | LEU | B | 540 | -9.487 | 0.803 | 23.239 | 1.00 | 18.23 |
| | ATOM | 3750 | CA | LEU | B | 540 | -8.743 | -0.048 | 22.319 | 1.00 | 18.05 |
| | ATOM | 3751 | CB | LEU | B | 540 | -8.909 | -1.528 | 22.701 | 1.00 | 16.38 |
| | ATOM | 3752 | CG | LEU | B | 540 | -8.188 | -2.554 | 21.821 | 1.00 | 19.81 |
| | ATOM | 3753 | CD1 | LEU | B | 540 | -6.679 | -2.303 | 21.828 | 1.00 | 19.27 |
| 10 | ATOM | 3754 | CD2 | LEU | B | 540 | -8.473 | -3.952 | 22.327 | 1.00 | 18.00 |
| | ATOM | 3755 | C | LEU | B | 540 | -9.241 | 0.169 | 20.891 | 1.00 | 21.50 |
| | ATOM | 3756 | O | LEU | B | 540 | -8.449 | 0.293 | 19.964 | 1.00 | 20.41 |
| | ATOM | 3757 | N | LEU | B | 541 | -10.559 | 0.206 | 20.726 | 1.00 | 22.40 |
| | ATOM | 3758 | CA | LEU | B | 541 | -11.164 | 0.419 | 19.413 | 1.00 | 23.27 |
| 15 | ATOM | 3759 | CB | LEU | B | 541 | -12.686 | 0.429 | 19.527 | 1.00 | 25.12 |
| | ATOM | 3760 | CG | LEU | B | 541 | -13.410 | -0.808 | 18.999 | 1.00 | 36.53 |
| | ATOM | 3761 | CD1 | LEU | B | 541 | -14.910 | -0.671 | 19.273 | 1.00 | 30.98 |
| | ATOM | 3762 | CD2 | LEU | B | 541 | -13.136 | -0.971 | 17.508 | 1.00 | 31.93 |
| | ATOM | 3763 | C | LEU | B | 541 | -10.697 | 1.751 | 18.842 | 1.00 | 22.46 |
| 20 | ATOM | 3764 | O | LEU | B | 541 | -10.359 | 1.845 | 17.666 | 1.00 | 26.29 |
| | ATOM | 3765 | N | GLU | B | 542 | -10.694 | 2.781 | 19.680 | 1.00 | 23.96 |
| | ATOM | 3766 | CA | GLU | B | 542 | -10.248 | 4.106 | 19.270 | 1.00 | 26.91 |
| | ATOM | 3767 | CB | GLU | B | 542 | -10.250 | 5.050 | 20.468 | 1.00 | 30.84 |
| | ATOM | 3768 | CG | GLU | B | 542 | -11.166 | 6.245 | 20.347 | 1.00 | 37.20 |
| 25 | ATOM | 3769 | CD | GLU | B | 542 | -11.138 | 7.105 | 21.597 | 1.00 | 39.98 |
| | ATOM | 3770 | OE1 | GLU | B | 542 | -12.223 | 7.385 | 22.144 | 1.00 | 39.92 |
| | ATOM | 3771 | OE2 | GLU | B | 542 | -10.028 | 7.494 | 22.034 | 1.00 | 38.96 |
| | ATOM | 3772 | C | GLU | B | 542 | -8.826 | 4.010 | 18.724 | 1.00 | 27.90 |
| | ATOM | 3773 | O | GLU | B | 542 | -8.530 | 4.492 | 17.634 | 1.00 | 29.32 |
| 30 | ATOM | 3774 | N | MET | B | 543 | -7.945 | 3.388 | 19.499 | 1.00 | 26.41 |
| | ATOM | 3775 | CA | MET | B | 543 | -6.552 | 3.237 | 19.107 | 1.00 | 23.53 |
| | ATOM | 3776 | CB | MET | B | 543 | -5.749 | 2.591 | 20.247 | 1.00 | 24.60 |
| | ATOM | 3777 | CG | MET | B | 543 | -5.812 | 3.338 | 21.579 | 1.00 | 26.46 |
| | ATOM | 3778 | SD | MET | B | 543 | -5.373 | 5.084 | 21.467 | 1.00 | 29.45 |
| 35 | ATOM | 3779 | CE | MET | B | 543 | -3.585 | 4.971 | 21.349 | 1.00 | 25.43 |
| | ATOM | 3780 | C | MET | B | 543 | -6.403 | 2.407 | 17.832 | 1.00 | 25.80 |
| | ATOM | 3781 | O | MET | B | 543 | -5.535 | 2.686 | 17.004 | 1.00 | 23.59 |
| | ATOM | 3782 | N | LEU | B | 544 | -7.254 | 1.394 | 17.673 | 1.00 | 27.74 |
| | ATOM | 3783 | CA | LEU | B | 544 | -7.202 | 0.522 | 16.499 | 1.00 | 26.32 |
| 40 | ATOM | 3784 | CB | LEU | B | 544 | -8.069 | -0.721 | 16.719 | 1.00 | 26.75 |
| | ATOM | 3785 | CG | LEU | B | 544 | -8.274 | -1.632 | 15.502 | 1.00 | 28.12 |
| | ATOM | 3786 | CD1 | LEU | B | 544 | -6.956 | -2.294 | 15.136 | 1.00 | 26.36 |
| | ATOM | 3787 | CD2 | LEU | B | 544 | -9.330 | -2.680 | 15.803 | 1.00 | 27.00 |
| | ATOM | 3788 | C | LEU | B | 544 | -7.672 | 1.252 | 15.250 | 1.00 | 26.97 |
| 45 | ATOM | 3789 | O | LEU | B | 544 | -7.036 | 1.181 | 14.195 | 1.00 | 24.25 |
| | ATOM | 3790 | N | ASP | B | 545 | -8.787 | 1.961 | 15.372 | 1.00 | 30.37 |
| | ATOM | 3791 | CA | ASP | B | 545 | -9.338 | 2.702 | 14.244 | 1.00 | 32.34 |
| | ATOM | 3792 | CB | ASP | B | 545 | -10.668 | 3.346 | 14.637 | 1.00 | 36.61 |
| | ATOM | 3793 | CG | ASP | B | 545 | -11.818 | 2.370 | 14.565 | 1.00 | 42.73 |
| 50 | ATOM | 3794 | OD1 | ASP | B | 545 | -12.858 | 2.624 | 15.211 | 1.00 | 47.39 |
| | ATOM | 3795 | OD2 | ASP | B | 545 | -11.676 | 1.342 | 13.863 | 1.00 | 46.96 |
| | ATOM | 3796 | C | ASP | B | 545 | -8.382 | 3.762 | 13.711 | 1.00 | 31.27 |
| | ATOM | 3797 | O | ASP | B | 545 | -8.443 | 4.120 | 12.532 | 1.00 | 30.53 |
| | ATOM | 3798 | N | ALA | B | 546 | -7.506 | 4.272 | 14.572 | 1.00 | 29.02 |
| 55 | ATOM | 3799 | CA | ALA | B | 546 | -6.543 | 5.280 | 14.141 | 1.00 | 31.21 |
| | ATOM | 3800 | CB | ALA | B | 546 | -5.646 | 5.693 | 15.306 | 1.00 | 30.98 |
| | ATOM | 3801 | C | ALA | B | 546 | -5.697 | 4.731 | 12.996 | 1.00 | 32.14 |
| | ATOM | 3802 | O | ALA | B | 546 | -5.189 | 5.490 | 12.170 | 1.00 | 33.78 |
| | ATOM | 3803 | N | HIS | B | 547 | -5.555 | 3.410 | 12.943 | 1.00 | 32.27 |
| 60 | ATOM | 3804 | CA | HIS | B | 547 | -4.773 | 2.767 | 11.892 | 1.00 | 37.73 |
| | ATOM | 3805 | CB | HIS | B | 547 | -3.991 | 1.576 | 12.457 | 1.00 | 35.83 |

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|----|--------|------|-----|-----|---|-----|---------|---------|--------|------|-------|
| 5 | ATOM | 3806 | CG | HIS | B | 547 | -2.796 | 1.968 | 13.269 | 1.00 | 34.54 |
| | ATOM | 3807 | CD2 | HIS | B | 547 | -2.698 | 2.553 | 14.486 | 1.00 | 30.23 |
| | ATOM | 3808 | ND1 | HIS | B | 547 | -1.502 | 1.755 | 12.840 | 1.00 | 34.23 |
| | ATOM | 3809 | CE1 | HIS | B | 547 | -0.659 | 2.193 | 13.760 | 1.00 | 36.72 |
| | ATOM | 3810 | NE2 | HIS | B | 547 | -1.360 | 2.681 | 14.768 | 1.00 | 31.48 |
| 10 | ATOM | 3811 | C | HIS | B | 547 | -5.649 | 2.286 | 10.735 | 1.00 | 43.69 |
| | ATOM | 3812 | O | HIS | B | 547 | -5.178 | 2.152 | 9.606 | 1.00 | 46.04 |
| | ATOM | 3813 | N | ARG | B | 548 | -6.919 | 2.020 | 11.019 | 1.00 | 48.35 |
| | ATOM | 3814 | CA | ARG | B | 548 | -7.843 | 1.551 | 9.993 | 1.00 | 54.74 |
| | ATOM | 3815 | CB | ARG | B | 548 | -8.522 | 0.267 | 10.452 | 1.00 | 54.66 |
| 15 | ATOM | 3816 | C | ARG | B | 548 | -8.886 | 2.619 | 9.681 | 1.00 | 59.94 |
| | ATOM | 3817 | O | ARG | B | 548 | -8.580 | 3.812 | 9.672 | 1.00 | 62.81 |
| | ATOM | 3818 | N | LEU | B | 549 | -10.116 | 2.186 | 9.422 | 1.00 | 64.81 |
| | ATOM | 3819 | CA | LEU | B | 549 | -11.204 | 3.109 | 9.112 | 1.00 | 67.59 |
| | ATOM | 3820 | CB | LEU | B | 549 | -12.478 | 2.327 | 8.799 | 1.00 | 68.06 |
| 20 | ATOM | 3821 | C | LEU | B | 549 | -11.449 | 4.069 | 10.275 | 1.00 | 69.12 |
| | ATOM | 3822 | O | LEU | B | 549 | -11.451 | 5.297 | 10.036 | 1.00 | 68.96 |
| | ATOM | 3823 | OXT | LEU | B | 549 | -11.634 | 3.579 | 11.412 | 1.00 | 70.70 |
| | HETATM | 3824 | CP9 | DES | B | 600 | -4.547 | -6.077 | 22.000 | 1.00 | 18.55 |
| | HETATM | 3825 | CP8 | DES | B | 600 | -3.163 | -6.365 | 21.467 | 1.00 | 17.72 |
| 25 | HETATM | 3826 | CP7 | DES | B | 600 | -2.897 | -7.853 | 21.381 | 1.00 | 21.17 |
| | HETATM | 3827 | CP6 | DES | B | 600 | -3.719 | -8.551 | 20.374 | 1.00 | 22.05 |
| | HETATM | 3828 | CP1 | DES | B | 600 | -3.405 | -8.481 | 18.998 | 1.00 | 21.32 |
| | HETATM | 3829 | CP2 | DES | B | 600 | -4.239 | -9.095 | 18.063 | 1.00 | 21.61 |
| | HETATM | 3830 | CP3 | DES | B | 600 | -5.388 | -9.771 | 18.509 | 1.00 | 24.89 |
| 30 | HETATM | 3831 | OP3 | DES | B | 600 | -6.244 | -10.339 | 17.600 | 1.00 | 24.94 |
| | HETATM | 3832 | CP4 | DES | B | 600 | -5.718 | -9.858 | 19.860 | 1.00 | 24.08 |
| | HETATM | 3833 | CP5 | DES | B | 600 | -4.877 | -9.240 | 20.791 | 1.00 | 24.67 |
| | HETATM | 3834 | C7 | DES | B | 600 | -1.998 | -8.460 | 22.190 | 1.00 | 16.67 |
| | HETATM | 3835 | C6 | DES | B | 600 | -1.330 | -7.834 | 23.325 | 1.00 | 15.39 |
| 35 | HETATM | 3836 | C5 | DES | B | 600 | -2.054 | -7.642 | 24.522 | 1.00 | 17.62 |
| | HETATM | 3837 | C4 | DES | B | 600 | -1.433 | -7.072 | 25.634 | 1.00 | 16.16 |
| | HETATM | 3838 | C3 | DES | B | 600 | -0.077 | -6.685 | 25.542 | 1.00 | 20.04 |
| | HETATM | 3839 | O3 | DES | B | 600 | 0.509 | -6.113 | 26.655 | 1.00 | 15.55 |
| | HETATM | 3840 | C2 | DES | B | 600 | 0.669 | -6.866 | 24.353 | 1.00 | 18.94 |
| 40 | HETATM | 3841 | C1 | DES | B | 600 | 0.035 | -7.440 | 23.241 | 1.00 | 15.20 |
| | HETATM | 3842 | C8 | DES | B | 600 | -1.642 | -9.903 | 21.942 | 1.00 | 17.61 |
| | HETATM | 3843 | C9 | DES | B | 600 | -0.440 | -10.009 | 20.998 | 1.00 | 11.63 |
| | HETATM | 3844 | C1 | CBM | B | 417 | -4.997 | -22.994 | 25.273 | 1.00 | 55.80 |
| | HETATM | 3845 | O4 | CBM | B | 417 | -4.789 | -24.187 | 25.003 | 1.00 | 55.56 |
| 45 | HETATM | 3846 | O3 | CBM | B | 417 | -4.798 | -22.559 | 26.552 | 1.00 | 56.04 |
| | HETATM | 3847 | C2 | CBM | B | 417 | -5.468 | -21.960 | 24.264 | 1.00 | 57.04 |
| | HETATM | 3848 | C1 | CBM | B | 530 | -15.278 | -5.124 | 10.243 | 1.00 | 87.39 |
| | HETATM | 3849 | O4 | CBM | B | 530 | -15.852 | -5.086 | 9.064 | 1.00 | 87.68 |
| | HETATM | 3850 | O3 | CBM | B | 530 | -15.832 | -4.291 | 11.201 | 1.00 | 86.22 |
| 50 | HETATM | 3851 | C2 | CBM | B | 530 | -14.207 | -5.886 | 10.628 | 1.00 | 87.65 |
| | ATOM | 3852 | CB | HIS | C | 687 | 9.818 | -20.030 | -2.211 | 1.00 | 63.34 |
| | ATOM | 3853 | C | HIS | C | 687 | 10.133 | -20.267 | -4.689 | 1.00 | 63.49 |
| | ATOM | 3854 | O | HIS | C | 687 | 11.204 | -20.840 | -4.472 | 1.00 | 63.87 |
| | ATOM | 3855 | N | HIS | C | 687 | 7.944 | -19.563 | -3.758 | 1.00 | 65.42 |
| 55 | ATOM | 3856 | CA | HIS | C | 687 | 9.424 | -19.484 | -3.586 | 1.00 | 64.86 |
| | ATOM | 3857 | N | LYS | C | 688 | 9.533 | -20.281 | -5.875 | 1.00 | 62.00 |
| | ATOM | 3858 | CA | LYS | C | 688 | 10.101 | -20.999 | -7.009 | 1.00 | 60.81 |
| | ATOM | 3859 | CB | LYS | C | 688 | 8.980 | -21.540 | -7.901 | 1.00 | 61.76 |
| | ATOM | 3860 | C | LYS | C | 688 | 11.050 | -20.127 | -7.827 | 1.00 | 57.47 |
| 60 | ATOM | 3861 | O | LYS | C | 688 | 12.253 | -20.379 | -7.858 | 1.00 | 57.64 |
| | ATOM | 3862 | N | ILE | C | 689 | 10.511 | -19.103 | -8.482 | 1.00 | 55.74 |

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|----|------|------|-----|-----|---|-----|--------|---------|---------|------|-------|
| 5 | ATOM | 3863 | CA | ILE | C | 689 | 11.326 | -18.212 | -9.306 | 1.00 | 53.09 |
| | ATOM | 3864 | CB | ILE | C | 689 | 10.496 | -17.057 | -9.889 | 1.00 | 53.83 |
| | ATOM | 3865 | CG2 | ILE | C | 689 | 11.334 | -16.286 | -10.902 | 1.00 | 54.55 |
| | ATOM | 3866 | CG1 | ILE | C | 689 | 9.229 | -17.603 | -10.551 | 1.00 | 52.90 |
| | ATOM | 3867 | CD1 | ILE | C | 689 | 8.406 | -16.550 | -11.258 | 1.00 | 50.45 |
| 10 | ATOM | 3868 | C | ILE | C | 689 | 12.513 | -17.611 | -8.560 | 1.00 | 50.82 |
| | ATOM | 3869 | O | ILE | C | 689 | 13.616 | -17.550 | -9.097 | 1.00 | 51.28 |
| | ATOM | 3870 | N | LEU | C | 690 | 12.288 | -17.162 | -7.329 | 1.00 | 48.01 |
| | ATOM | 3871 | CA | LEU | C | 690 | 13.362 | -16.570 | -6.534 | 1.00 | 47.33 |
| | ATOM | 3872 | CB | LEU | C | 690 | 12.812 | -16.058 | -5.199 | 1.00 | 42.51 |
| 15 | ATOM | 3873 | CG | LEU | C | 690 | 13.835 | -15.501 | -4.206 | 1.00 | 40.67 |
| | ATOM | 3874 | CD1 | LEU | C | 690 | 14.575 | -14.324 | -4.831 | 1.00 | 39.95 |
| | ATOM | 3875 | CD2 | LEU | C | 690 | 13.128 | -15.078 | -2.926 | 1.00 | 38.77 |
| | ATOM | 3876 | C | LEU | C | 690 | 14.445 | -17.615 | -6.282 | 1.00 | 48.87 |
| | ATOM | 3877 | O | LEU | C | 690 | 15.643 | -17.340 | -6.393 | 1.00 | 46.71 |
| 20 | ATOM | 3878 | N | HIS | C | 691 | 14.001 | -18.818 | -5.939 | 1.00 | 51.36 |
| | ATOM | 3879 | CA | HIS | C | 691 | 14.886 | -19.946 | -5.675 | 1.00 | 53.35 |
| | ATOM | 3880 | CB | HIS | C | 691 | 14.042 | -21.203 | -5.460 | 1.00 | 58.64 |
| | ATOM | 3881 | CG | HIS | C | 691 | 14.655 | -22.195 | -4.526 | 1.00 | 62.94 |
| | ATOM | 3882 | CD2 | HIS | C | 691 | 15.503 | -23.227 | -4.751 | 1.00 | 64.95 |
| 25 | ATOM | 3883 | ND1 | HIS | C | 691 | 14.392 | -22.202 | -3.173 | 1.00 | 65.49 |
| | ATOM | 3884 | CE1 | HIS | C | 691 | 15.053 | -23.195 | -2.605 | 1.00 | 68.18 |
| | ATOM | 3885 | NE2 | HIS | C | 691 | 15.733 | -23.833 | -3.540 | 1.00 | 68.77 |
| | ATOM | 3886 | C | HIS | C | 691 | 15.824 | -20.162 | -6.861 | 1.00 | 52.19 |
| | ATOM | 3887 | O | HIS | C | 691 | 17.048 | -20.153 | -6.717 | 1.00 | 47.53 |
| 30 | ATOM | 3888 | N | ARG | C | 692 | 15.222 | -20.350 | -8.032 | 1.00 | 52.37 |
| | ATOM | 3889 | CA | ARG | C | 692 | 15.949 | -20.586 | -9.271 | 1.00 | 52.90 |
| | ATOM | 3890 | CB | ARG | C | 692 | 14.955 | -20.832 | -10.410 | 1.00 | 54.04 |
| | ATOM | 3891 | CG | ARG | C | 692 | 15.575 | -20.826 | -11.797 | 1.00 | 57.52 |
| | ATOM | 3892 | CD | ARG | C | 692 | 14.528 | -21.048 | -12.874 | 1.00 | 58.25 |
| 35 | ATOM | 3893 | NE | ARG | C | 692 | 14.375 | -19.878 | -13.732 | 1.00 | 61.43 |
| | ATOM | 3894 | CZ | ARG | C | 692 | 13.218 | -19.260 | -13.951 | 1.00 | 64.32 |
| | ATOM | 3895 | NH1 | ARG | C | 692 | 12.108 | -19.706 | -13.378 | 1.00 | 63.22 |
| | ATOM | 3896 | NH2 | ARG | C | 692 | 13.171 | -18.197 | -14.746 | 1.00 | 65.93 |
| | ATOM | 3897 | C | ARG | C | 692 | 16.873 | -19.434 | -9.639 | 1.00 | 53.09 |
| 40 | ATOM | 3898 | O | ARG | C | 692 | 18.047 | -19.644 | -9.956 | 1.00 | 53.06 |
| | ATOM | 3899 | N | LEU | C | 693 | 16.338 | -18.217 | -9.607 | 1.00 | 50.73 |
| | ATOM | 3900 | CA | LEU | C | 693 | 17.125 | -17.039 | -9.945 | 1.00 | 49.53 |
| | ATOM | 3901 | CB | LEU | C | 693 | 16.249 | -15.784 | -9.881 | 1.00 | 49.56 |
| | ATOM | 3902 | CG | LEU | C | 693 | 15.781 | -15.245 | -11.239 | 1.00 | 49.78 |
| 45 | ATOM | 3903 | CD1 | LEU | C | 693 | 15.219 | -16.389 | -12.079 | 1.00 | 50.30 |
| | ATOM | 3904 | CD2 | LEU | C | 693 | 14.728 | -14.170 | -11.037 | 1.00 | 48.79 |
| | ATOM | 3905 | C | LEU | C | 693 | 18.318 | -16.904 | -9.006 | 1.00 | 48.38 |
| | ATOM | 3906 | O | LEU | C | 693 | 19.382 | -16.426 | -9.402 | 1.00 | 46.35 |
| | ATOM | 3907 | N | LEU | C | 694 | 18.135 | -17.329 | -7.761 | 1.00 | 46.74 |
| 50 | ATOM | 3908 | CA | LEU | C | 694 | 19.204 | -17.272 | -6.775 | 1.00 | 49.41 |
| | ATOM | 3909 | CB | LEU | C | 694 | 18.634 | -17.415 | -5.362 | 1.00 | 45.20 |
| | ATOM | 3910 | CG | LEU | C | 694 | 18.222 | -16.128 | -4.643 | 1.00 | 40.19 |
| | ATOM | 3911 | CD1 | LEU | C | 694 | 17.456 | -16.474 | -3.371 | 1.00 | 41.65 |
| | ATOM | 3912 | CD2 | LEU | C | 694 | 19.453 | -15.307 | -4.317 | 1.00 | 35.91 |
| 55 | ATOM | 3913 | C | LEU | C | 694 | 20.172 | -18.417 | -7.058 | 1.00 | 54.15 |
| | ATOM | 3914 | O | LEU | C | 694 | 21.370 | -18.320 | -6.776 | 1.00 | 53.55 |
| | ATOM | 3915 | N | GLN | C | 695 | 19.634 | -19.498 | -7.619 | 1.00 | 57.44 |
| | ATOM | 3916 | CA | GLN | C | 695 | 20.416 | -20.685 | -7.959 | 1.00 | 62.46 |
| | ATOM | 3917 | CB | GLN | C | 695 | 19.477 | -21.853 | -8.304 | 1.00 | 61.95 |
| 60 | ATOM | 3918 | CG | GLN | C | 695 | 19.548 | -23.010 | -7.311 | 1.00 | 61.49 |
| | ATOM | 3919 | CD | GLN | C | 695 | 18.454 | -24.053 | -7.490 | 1.00 | 62.78 |

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|----|------|------|-----|-----|---|-----|---------|---------|---------|------|-------|
| 5 | ATOM | 3920 | OE1 | GLN | C | 695 | 18.262 | -24.928 | -6.653 | 1.00 | 63.33 |
| | ATOM | 3921 | NE2 | GLN | C | 695 | 17.720 | -23.969 | -8.608 | 1.00 | 60.37 |
| | ATOM | 3922 | C | GLN | C | 695 | 21.330 | -20.414 | -9.149 | 1.00 | 65.13 |
| | ATOM | 3923 | O | GLN | C | 695 | 22.517 | -20.740 | -9.116 | 1.00 | 65.87 |
| | ATOM | 3924 | N | ASP | C | 696 | 20.761 | -19.824 | -10.197 | 1.00 | 67.67 |
| 10 | ATOM | 3925 | CA | ASP | C | 696 | 21.492 | -19.500 | -11.420 | 1.00 | 70.66 |
| | ATOM | 3926 | CB | ASP | C | 696 | 20.801 | -18.348 | -12.151 | 1.00 | 71.06 |
| | ATOM | 3927 | CG | ASP | C | 696 | 20.127 | -18.792 | -13.430 | 1.00 | 71.70 |
| | ATOM | 3928 | OD1 | ASP | C | 696 | 20.637 | -18.455 | -14.521 | 1.00 | 72.47 |
| | ATOM | 3929 | OD2 | ASP | C | 696 | 19.086 | -19.478 | -13.342 | 1.00 | 71.41 |
| 15 | ATOM | 3930 | C | ASP | C | 696 | 22.951 | -19.132 | -11.169 | 1.00 | 72.41 |
| | ATOM | 3931 | O | ASP | C | 696 | 23.245 | -18.115 | -10.541 | 1.00 | 72.56 |
| | ATOM | 3932 | N | SER | C | 697 | 23.859 | -19.967 | -11.668 | 1.00 | 74.67 |
| | ATOM | 3933 | CA | SER | C | 697 | 25.291 | -19.741 | -11.507 | 1.00 | 76.45 |
| | ATOM | 3934 | CB | SER | C | 697 | 26.019 | -21.076 | -11.377 | 1.00 | 76.00 |
| 20 | ATOM | 3935 | C | SER | C | 697 | 25.841 | -18.960 | -12.696 | 1.00 | 78.44 |
| | ATOM | 3936 | O | SER | C | 697 | 26.286 | -17.809 | -12.489 | 1.00 | 79.20 |
| | ATOM | 3937 | OXT | SER | C | 697 | 25.818 | -19.510 | -13.820 | 1.00 | 80.07 |
| | ATOM | 3938 | CB | LYS | D | 686 | -14.070 | 13.661 | 16.843 | 1.00 | 50.28 |
| | ATOM | 3939 | C | LYS | D | 686 | -13.682 | 14.418 | 19.199 | 1.00 | 51.59 |
| 25 | ATOM | 3940 | O | LYS | D | 686 | -12.629 | 14.738 | 19.759 | 1.00 | 50.42 |
| | ATOM | 3941 | N | LYS | D | 686 | -12.910 | 15.796 | 17.283 | 1.00 | 50.43 |
| | ATOM | 3942 | CA | LYS | D | 686 | -13.976 | 14.872 | 17.769 | 1.00 | 50.62 |
| | ATOM | 3943 | N | HIS | D | 687 | -14.617 | 13.676 | 19.787 | 1.00 | 49.91 |
| | ATOM | 3944 | CA | HIS | D | 687 | -14.447 | 13.176 | 21.144 | 1.00 | 51.28 |
| 30 | ATOM | 3945 | CB | HIS | D | 687 | -15.806 | 12.984 | 21.828 | 1.00 | 54.12 |
| | ATOM | 3946 | CG | HIS | D | 687 | -15.713 | 12.336 | 23.177 | 1.00 | 60.06 |
| | ATOM | 3947 | CD2 | HIS | D | 687 | -15.418 | 11.064 | 23.539 | 1.00 | 61.05 |
| | ATOM | 3948 | ND1 | HIS | D | 687 | -15.911 | 13.030 | 24.352 | 1.00 | 62.39 |
| | ATOM | 3949 | CE1 | HIS | D | 687 | -15.741 | 12.215 | 25.378 | 1.00 | 62.76 |
| 35 | ATOM | 3950 | NE2 | HIS | D | 687 | -15.441 | 11.016 | 24.912 | 1.00 | 63.46 |
| | ATOM | 3951 | C | HIS | D | 687 | -13.691 | 11.849 | 21.163 | 1.00 | 49.55 |
| | ATOM | 3952 | O | HIS | D | 687 | -14.099 | 10.878 | 20.524 | 1.00 | 50.84 |
| | ATOM | 3953 | N | LYS | D | 688 | -12.593 | 11.816 | 21.909 | 1.00 | 44.00 |
| | ATOM | 3954 | CA | LYS | D | 688 | -11.784 | 10.611 | 22.038 | 1.00 | 40.31 |
| 40 | ATOM | 3955 | CB | LYS | D | 688 | -10.446 | 10.773 | 21.299 | 1.00 | 41.42 |
| | ATOM | 3956 | CG | LYS | D | 688 | -10.513 | 10.595 | 19.780 | 1.00 | 42.76 |
| | ATOM | 3957 | CD | LYS | D | 688 | -9.123 | 10.716 | 19.152 | 1.00 | 38.66 |
| | ATOM | 3958 | CE | LYS | D | 688 | -9.162 | 10.529 | 17.640 | 1.00 | 38.28 |
| | ATOM | 3959 | NZ | LYS | D | 688 | -7.894 | 10.970 | 16.986 | 1.00 | 31.58 |
| 45 | ATOM | 3960 | C | LYS | D | 688 | -11.506 | 10.378 | 23.517 | 1.00 | 36.70 |
| | ATOM | 3961 | O | LYS | D | 688 | -11.271 | 11.326 | 24.266 | 1.00 | 33.38 |
| | ATOM | 3962 | N | ILE | D | 689 | -11.549 | 9.122 | 23.942 | 1.00 | 33.06 |
| | ATOM | 3963 | CA | ILE | D | 689 | -11.255 | 8.806 | 25.328 | 1.00 | 28.70 |
| | ATOM | 3964 | CB | ILE | D | 689 | -11.438 | 7.301 | 25.607 | 1.00 | 30.88 |
| 50 | ATOM | 3965 | CG2 | ILE | D | 689 | -10.725 | 6.912 | 26.899 | 1.00 | 31.45 |
| | ATOM | 3966 | CG1 | ILE | D | 689 | -12.927 | 6.971 | 25.721 | 1.00 | 32.57 |
| | ATOM | 3967 | CD1 | ILE | D | 689 | -13.308 | 5.679 | 25.031 | 1.00 | 29.79 |
| | ATOM | 3968 | C | ILE | D | 689 | -9.790 | 9.193 | 25.541 | 1.00 | 27.64 |
| | ATOM | 3969 | O | ILE | D | 689 | -9.405 | 9.649 | 26.611 | 1.00 | 25.54 |
| 55 | ATOM | 3970 | N | LEU | D | 690 | -8.985 | 9.021 | 24.496 | 1.00 | 24.25 |
| | ATOM | 3971 | CA | LEU | D | 690 | -7.563 | 9.348 | 24.549 | 1.00 | 26.63 |
| | ATOM | 3972 | CB | LEU | D | 690 | -6.903 | 9.021 | 23.200 | 1.00 | 22.83 |
| | ATOM | 3973 | CG | LEU | D | 690 | -5.433 | 9.387 | 22.992 | 1.00 | 25.47 |
| | ATOM | 3974 | CD1 | LEU | D | 690 | -4.595 | 8.772 | 24.108 | 1.00 | 24.03 |
| 60 | ATOM | 3975 | CD2 | LEU | D | 690 | -4.956 | 8.898 | 21.616 | 1.00 | 20.87 |
| | ATOM | 3976 | C | LEU | D | 690 | -7.344 | 10.823 | 24.902 | 1.00 | 26.64 |

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|----|--------|------|-----|-----|---|-----|---------|--------|--------|------|-------|
| 5 | ATOM | 3977 | O | LEU | D | 690 | -6.408 | 11.165 | 25.625 | 1.00 | 28.34 |
| | ATOM | 3978 | N | HIS | D | 691 | -8.206 | 11.694 | 24.383 | 1.00 | 27.77 |
| | ATOM | 3979 | CA | HIS | D | 691 | -8.107 | 13.125 | 24.665 | 1.00 | 29.16 |
| | ATOM | 3980 | CB | HIS | D | 691 | -9.156 | 13.907 | 23.861 | 1.00 | 30.89 |
| | ATOM | 3981 | CG | HIS | D | 691 | -8.903 | 13.935 | 22.386 | 1.00 | 37.09 |
| 10 | ATOM | 3982 | CD2 | HIS | D | 691 | -7.750 | 14.000 | 21.679 | 1.00 | 41.39 |
| | ATOM | 3983 | ND1 | HIS | D | 691 | -9.920 | 13.906 | 21.458 | 1.00 | 41.65 |
| | ATOM | 3984 | CE1 | HIS | D | 691 | -9.407 | 13.953 | 20.242 | 1.00 | 44.64 |
| | ATOM | 3985 | NE2 | HIS | D | 691 | -8.091 | 14.010 | 20.347 | 1.00 | 41.94 |
| | ATOM | 3986 | C | HIS | D | 691 | -8.338 | 13.373 | 26.159 | 1.00 | 26.65 |
| 15 | ATOM | 3987 | O | HIS | D | 691 | -7.602 | 14.120 | 26.802 | 1.00 | 24.50 |
| | ATOM | 3988 | N | ARG | D | 692 | -9.371 | 12.742 | 26.703 | 1.00 | 25.70 |
| | ATOM | 3989 | CA | ARG | D | 692 | -9.691 | 12.912 | 28.114 | 1.00 | 29.11 |
| | ATOM | 3990 | CB | ARG | D | 692 | -10.959 | 12.134 | 28.472 | 1.00 | 30.84 |
| | ATOM | 3991 | CG | ARG | D | 692 | -11.255 | 12.129 | 29.963 | 1.00 | 41.63 |
| 20 | ATOM | 3992 | CD | ARG | D | 692 | -12.502 | 11.327 | 30.290 | 1.00 | 48.83 |
| | ATOM | 3993 | NE | ARG | D | 692 | -13.618 | 12.198 | 30.647 | 1.00 | 54.50 |
| | ATOM | 3994 | CZ | ARG | D | 692 | -14.498 | 12.677 | 29.774 | 1.00 | 59.37 |
| | ATOM | 3995 | NH1 | ARG | D | 692 | -14.392 | 12.371 | 28.486 | 1.00 | 60.97 |
| | ATOM | 3996 | NH2 | ARG | D | 692 | -15.483 | 13.464 | 30.188 | 1.00 | 59.07 |
| 25 | ATOM | 3997 | C | ARG | D | 692 | -8.548 | 12.451 | 29.011 | 1.00 | 28.30 |
| | ATOM | 3998 | O | ARG | D | 692 | -8.139 | 13.167 | 29.929 | 1.00 | 26.50 |
| | ATOM | 3999 | N | LEU | D | 693 | -8.030 | 11.259 | 28.737 | 1.00 | 24.87 |
| | ATOM | 4000 | CA | LEU | D | 693 | -6.943 | 10.705 | 29.536 | 1.00 | 27.17 |
| | ATOM | 4001 | CB | LEU | D | 693 | -6.674 | 9.254 | 29.116 | 1.00 | 28.45 |
| 30 | ATOM | 4002 | CG | LEU | D | 693 | -7.844 | 8.300 | 29.391 | 1.00 | 30.40 |
| | ATOM | 4003 | CD1 | LEU | D | 693 | -7.575 | 6.932 | 28.778 | 1.00 | 34.79 |
| | ATOM | 4004 | CD2 | LEU | D | 693 | -8.043 | 8.171 | 30.894 | 1.00 | 32.02 |
| | ATOM | 4005 | C | LEU | D | 693 | -5.670 | 11.539 | 29.440 | 1.00 | 25.96 |
| | ATOM | 4006 | O | LEU | D | 693 | -4.948 | 11.700 | 30.428 | 1.00 | 27.01 |
| 35 | ATOM | 4007 | N | LEU | D | 694 | -5.395 | 12.080 | 28.257 | 1.00 | 25.33 |
| | ATOM | 4008 | CA | LEU | D | 694 | -4.207 | 12.906 | 28.062 | 1.00 | 27.22 |
| | ATOM | 4009 | CB | LEU | D | 694 | -3.948 | 13.126 | 26.572 | 1.00 | 24.61 |
| | ATOM | 4010 | CG | LEU | D | 694 | -3.118 | 12.080 | 25.825 | 1.00 | 22.20 |
| | ATOM | 4011 | CD1 | LEU | D | 694 | -3.230 | 12.332 | 24.324 | 1.00 | 21.13 |
| 40 | ATOM | 4012 | CD2 | LEU | D | 694 | -1.666 | 12.148 | 26.275 | 1.00 | 21.34 |
| | ATOM | 4013 | C | LEU | D | 694 | -4.336 | 14.270 | 28.742 | 1.00 | 32.40 |
| | ATOM | 4014 | O | LEU | D | 694 | -3.339 | 14.889 | 29.102 | 1.00 | 31.55 |
| | ATOM | 4015 | N | GLN | D | 695 | -5.570 | 14.733 | 28.915 | 1.00 | 36.93 |
| | ATOM | 4016 | CA | GLN | D | 695 | -5.820 | 16.032 | 29.528 | 1.00 | 43.18 |
| 45 | ATOM | 4017 | CB | GLN | D | 695 | -7.022 | 16.694 | 28.862 | 1.00 | 40.48 |
| | ATOM | 4018 | CG | GLN | D | 695 | -6.772 | 17.071 | 27.422 | 1.00 | 37.99 |
| | ATOM | 4019 | CD | GLN | D | 695 | -7.943 | 17.764 | 26.795 | 1.00 | 35.86 |
| | ATOM | 4020 | OE1 | GLN | D | 695 | -7.863 | 18.895 | 26.342 | 1.00 | 38.84 |
| | ATOM | 4021 | NE2 | GLN | D | 695 | -9.082 | 17.060 | 26.757 | 1.00 | 31.62 |
| 50 | ATOM | 4022 | C | GLN | D | 695 | -6.049 | 16.009 | 31.034 | 1.00 | 48.74 |
| | ATOM | 4023 | O | GLN | D | 695 | -6.119 | 17.065 | 31.660 | 1.00 | 51.25 |
| | ATOM | 4024 | N | ASP | D | 696 | -6.175 | 14.818 | 31.611 | 1.00 | 54.01 |
| | ATOM | 4025 | CA | ASP | D | 696 | -6.398 | 14.702 | 33.047 | 1.00 | 62.23 |
| | ATOM | 4026 | CB | ASP | D | 696 | -6.217 | 13.238 | 33.485 | 1.00 | 63.97 |
| 55 | ATOM | 4027 | CG | ASP | D | 696 | -7.527 | 12.467 | 33.475 | 1.00 | 67.72 |
| | ATOM | 4028 | OD1 | ASP | D | 696 | -8.528 | 12.996 | 32.941 | 1.00 | 68.11 |
| | ATOM | 4029 | OD2 | ASP | D | 696 | -7.552 | 11.333 | 34.003 | 1.00 | 68.95 |
| | ATOM | 4030 | C | ASP | D | 696 | -5.456 | 15.622 | 33.840 | 1.00 | 65.60 |
| | ATOM | 4031 | O | ASP | D | 696 | -4.312 | 15.189 | 34.134 | 1.00 | 68.33 |
| 60 | ATOM | 4032 | OXT | ASP | D | 696 | -5.874 | 16.755 | 34.140 | 1.00 | 69.20 |
| | HETATM | 4033 | O | HOH | | 1 | 16.153 | -0.605 | -4.425 | 1.00 | 17.11 |

| | | | | | | | | | | |
|----|--------|------|---|-----|----|--------|---------|---------|------|-------|
| 5 | HETATM | 4034 | O | HOH | 2 | 16.570 | -5.304 | -16.560 | 1.00 | 21.44 |
| | HETATM | 4035 | O | HOH | 3 | 18.526 | 0.742 | -4.495 | 1.00 | 23.43 |
| | HETATM | 4036 | O | HOH | 4 | 13.647 | -2.187 | 8.588 | 1.00 | 25.82 |
| | HETATM | 4037 | O | HOH | 5 | 9.778 | -5.825 | 2.509 | 1.00 | 20.58 |
| | HETATM | 4038 | O | HOH | 6 | 17.072 | -3.605 | -8.015 | 1.00 | 18.38 |
| 10 | HETATM | 4039 | O | HOH | 7 | 24.920 | -1.689 | -2.780 | 1.00 | 25.74 |
| | HETATM | 4040 | O | HOH | 8 | 7.321 | -5.649 | 5.061 | 1.00 | 24.11 |
| | HETATM | 4041 | O | HOH | 9 | 25.976 | -3.535 | 15.158 | 1.00 | 26.78 |
| | HETATM | 4042 | O | HOH | 10 | 15.088 | -7.006 | -15.192 | 1.00 | 19.64 |
| | HETATM | 4043 | O | HOH | 11 | 14.070 | 0.925 | -5.953 | 1.00 | 20.55 |
| 15 | HETATM | 4044 | O | HOH | 12 | 18.008 | 3.407 | -6.654 | 1.00 | 32.30 |
| | HETATM | 4045 | O | HOH | 13 | 31.949 | -8.393 | 13.487 | 1.00 | 30.64 |
| | HETATM | 4046 | O | HOH | 14 | 19.625 | -2.804 | -4.279 | 1.00 | 24.45 |
| | HETATM | 4047 | O | HOH | 15 | 11.741 | 1.079 | -21.140 | 1.00 | 25.87 |
| | HETATM | 4048 | O | HOH | 16 | 25.067 | 13.951 | 14.153 | 1.00 | 31.07 |
| 20 | HETATM | 4049 | O | HOH | 17 | 15.501 | 1.323 | -10.393 | 1.00 | 21.01 |
| | HETATM | 4050 | O | HOH | 18 | 13.880 | 3.349 | -11.482 | 1.00 | 24.28 |
| | HETATM | 4051 | O | HOH | 19 | 17.591 | 0.979 | -8.828 | 1.00 | 35.26 |
| | HETATM | 4052 | O | HOH | 20 | 23.682 | -2.041 | -0.314 | 1.00 | 37.90 |
| | HETATM | 4053 | O | HOH | 21 | 15.754 | 9.496 | 11.841 | 1.00 | 39.44 |
| 25 | HETATM | 4054 | O | HOH | 22 | -4.943 | 7.574 | -3.066 | 1.00 | 37.67 |
| | HETATM | 4055 | O | HOH | 23 | 6.877 | 0.354 | -15.982 | 1.00 | 36.92 |
| | HETATM | 4056 | O | HOH | 24 | 15.806 | -4.002 | 8.671 | 1.00 | 30.38 |
| | HETATM | 4057 | O | HOH | 25 | 17.185 | -3.158 | -5.321 | 1.00 | 28.89 |
| | HETATM | 4058 | O | HOH | 26 | 17.572 | 9.249 | 17.009 | 1.00 | 30.15 |
| 30 | HETATM | 4059 | O | HOH | 27 | 24.096 | -2.929 | 11.604 | 1.00 | 31.37 |
| | HETATM | 4060 | O | HOH | 28 | 22.324 | -5.871 | -11.980 | 1.00 | 32.74 |
| | HETATM | 4061 | O | HOH | 29 | 27.547 | -12.361 | -0.801 | 1.00 | 36.61 |
| | HETATM | 4062 | O | HOH | 30 | 11.173 | 13.442 | -2.719 | 1.00 | 35.41 |
| | HETATM | 4063 | O | HOH | 31 | 15.438 | -9.527 | 5.483 | 1.00 | 29.88 |
| 35 | HETATM | 4064 | O | HOH | 32 | 9.946 | -6.564 | 5.983 | 1.00 | 35.05 |
| | HETATM | 4065 | O | HOH | 33 | 7.599 | 11.680 | -15.261 | 1.00 | 38.68 |
| | HETATM | 4066 | O | HOH | 34 | 20.112 | 10.503 | -5.109 | 1.00 | 42.66 |
| | HETATM | 4067 | O | HOH | 35 | 15.972 | 10.343 | 14.897 | 1.00 | 41.73 |
| | HETATM | 4068 | O | HOH | 36 | 22.401 | -5.914 | -9.527 | 1.00 | 28.08 |
| 40 | HETATM | 4069 | O | HOH | 37 | 16.128 | -0.899 | -8.109 | 1.00 | 33.13 |
| | HETATM | 4070 | O | HOH | 38 | 3.581 | 15.655 | -3.706 | 1.00 | 41.37 |
| | HETATM | 4071 | O | HOH | 39 | 31.900 | 13.545 | 21.339 | 1.00 | 37.79 |
| | HETATM | 4072 | O | HOH | 40 | 20.058 | -7.530 | 14.119 | 1.00 | 47.51 |
| | HETATM | 4073 | O | HOH | 41 | 34.634 | 6.668 | 15.632 | 1.00 | 29.24 |
| 45 | HETATM | 4074 | O | HOH | 42 | 17.968 | 10.511 | -9.085 | 1.00 | 44.60 |
| | HETATM | 4075 | O | HOH | 43 | 23.258 | -17.325 | -4.088 | 1.00 | 44.10 |
| | HETATM | 4076 | O | HOH | 44 | 4.034 | -1.472 | 27.521 | 1.00 | 15.22 |
| | HETATM | 4077 | O | HOH | 45 | -5.943 | -0.018 | 36.088 | 1.00 | 21.11 |
| | HETATM | 4078 | O | HOH | 46 | 6.084 | -1.509 | 29.478 | 1.00 | 19.51 |
| 50 | HETATM | 4079 | O | HOH | 47 | 9.762 | 1.061 | 15.621 | 1.00 | 27.74 |
| | HETATM | 4080 | O | HOH | 48 | 1.804 | 0.717 | 17.260 | 1.00 | 20.97 |
| | HETATM | 4081 | O | HOH | 49 | 0.929 | 0.421 | 30.281 | 1.00 | 19.64 |
| | HETATM | 4082 | O | HOH | 50 | 9.627 | 4.271 | 31.231 | 1.00 | 19.02 |
| | HETATM | 4083 | O | HOH | 51 | 2.121 | -0.261 | 13.654 | 1.00 | 26.09 |
| 55 | HETATM | 4084 | O | HOH | 52 | 20.060 | 10.275 | 17.711 | 1.00 | 25.49 |
| | HETATM | 4085 | O | HOH | 53 | -6.786 | 0.736 | 33.483 | 1.00 | 22.34 |
| | HETATM | 4086 | O | HOH | 54 | 2.751 | -4.136 | 27.760 | 1.00 | 19.93 |
| | HETATM | 4087 | O | HOH | 55 | 5.994 | -4.079 | 31.292 | 1.00 | 32.27 |
| | HETATM | 4088 | O | HOH | 56 | 19.416 | 16.921 | 21.645 | 1.00 | 25.54 |
| 60 | HETATM | 4089 | O | HOH | 57 | 4.833 | 2.325 | 29.006 | 1.00 | 19.00 |
| | HETATM | 4090 | O | HOH | 58 | -7.638 | -8.931 | 37.809 | 1.00 | 24.79 |

| | | | | | | | | | | |
|----|--------|------|---|-----|-----|---------|---------|--------|------|-------|
| 5 | HETATM | 4091 | O | HOH | 59 | 28.442 | -4.673 | 21.875 | 1.00 | 24.32 |
| | HETATM | 4092 | O | HOH | 60 | 1.094 | -4.893 | 32.100 | 1.00 | 24.27 |
| | HETATM | 4093 | O | HOH | 61 | 0.905 | -7.306 | 32.783 | 1.00 | 21.33 |
| | HETATM | 4094 | O | HOH | 62 | 3.396 | -2.971 | 32.306 | 1.00 | 26.13 |
| | HETATM | 4095 | O | HOH | 63 | 10.363 | 4.576 | 28.391 | 1.00 | 33.43 |
| 10 | HETATM | 4096 | O | HOH | 64 | 19.551 | -6.473 | 16.597 | 1.00 | 35.38 |
| | HETATM | 4097 | O | HOH | 65 | -2.888 | -19.627 | 15.665 | 1.00 | 27.99 |
| | HETATM | 4098 | O | HOH | 66 | -7.275 | -9.745 | 31.077 | 1.00 | 27.00 |
| | HETATM | 4099 | O | HOH | 67 | 10.189 | 3.580 | 16.510 | 1.00 | 24.19 |
| | HETATM | 4100 | O | HOH | 68 | 2.741 | 0.716 | 28.382 | 1.00 | 16.48 |
| 15 | HETATM | 4101 | O | HOH | 69 | 23.522 | -4.323 | 13.943 | 1.00 | 27.48 |
| | HETATM | 4102 | O | HOH | 70 | 17.133 | 8.133 | 19.686 | 1.00 | 32.24 |
| | HETATM | 4103 | O | HOH | 71 | -0.295 | 4.535 | 35.884 | 1.00 | 33.42 |
| | HETATM | 4104 | O | HOH | 72 | 9.519 | 10.828 | 34.842 | 1.00 | 29.38 |
| | HETATM | 4105 | O | HOH | 73 | 6.291 | 14.878 | 29.070 | 1.00 | 28.21 |
| 20 | HETATM | 4106 | O | HOH | 74 | -1.721 | 6.480 | 13.381 | 1.00 | 49.91 |
| | HETATM | 4107 | O | HOH | 75 | 10.091 | -15.427 | 26.194 | 1.00 | 24.17 |
| | HETATM | 4108 | O | HOH | 76 | 5.029 | 7.461 | 17.718 | 1.00 | 18.91 |
| | HETATM | 4109 | O | HOH | 77 | 3.758 | 2.086 | 14.306 | 1.00 | 28.28 |
| | HETATM | 4110 | O | HOH | 78 | -1.390 | -18.739 | 33.183 | 1.00 | 41.11 |
| 25 | HETATM | 4111 | O | HOH | 79 | 12.703 | -8.687 | 32.119 | 1.00 | 36.21 |
| | HETATM | 4112 | O | HOH | 80 | 22.270 | -6.451 | 14.844 | 1.00 | 33.21 |
| | HETATM | 4113 | O | HOH | 81 | 1.458 | 4.605 | 34.026 | 1.00 | 23.59 |
| | HETATM | 4114 | O | HOH | 82 | 1.759 | -2.158 | 30.374 | 1.00 | 28.78 |
| | HETATM | 4115 | O | HOH | 83 | 6.153 | -21.372 | 23.188 | 1.00 | 31.14 |
| 30 | HETATM | 4116 | O | HOH | 84 | 36.525 | 0.463 | 20.792 | 1.00 | 45.26 |
| | HETATM | 4117 | O | HOH | 85 | 13.832 | 9.696 | 13.792 | 1.00 | 33.12 |
| | HETATM | 4118 | O | HOH | 86 | 31.166 | 6.635 | 24.924 | 1.00 | 35.19 |
| | HETATM | 4119 | O | HOH | 87 | 8.844 | -10.389 | 34.180 | 1.00 | 48.80 |
| | HETATM | 4120 | O | HOH | 88 | 9.581 | -6.956 | 34.136 | 1.00 | 42.95 |
| 35 | HETATM | 4121 | O | HOH | 89 | -1.563 | 15.887 | 27.596 | 1.00 | 39.35 |
| | HETATM | 4122 | O | HOH | 90 | -5.286 | 10.345 | 32.757 | 1.00 | 35.20 |
| | HETATM | 4123 | O | HOH | 91 | 15.035 | 0.607 | 13.339 | 1.00 | 29.53 |
| | HETATM | 4124 | O | HOH | 92 | -10.984 | -1.500 | 30.272 | 1.00 | 29.84 |
| | HETATM | 4125 | O | HOH | 93 | -7.239 | -0.271 | -1.207 | 1.00 | 48.98 |
| 40 | HETATM | 4126 | O | HOH | 94 | 18.022 | -4.902 | 34.286 | 1.00 | 35.28 |
| | HETATM | 4127 | O | HOH | 95 | 29.347 | -6.319 | 19.920 | 1.00 | 37.20 |
| | HETATM | 4128 | O | HOH | 96 | -14.309 | -19.369 | 20.945 | 1.00 | 30.23 |
| | HETATM | 4129 | O | HOH | 97 | 31.496 | 4.614 | 18.716 | 1.00 | 38.79 |
| | HETATM | 4130 | O | HOH | 98 | 26.567 | 9.759 | 25.629 | 1.00 | 29.72 |
| 45 | HETATM | 4131 | O | HOH | 99 | 2.848 | 14.531 | 1.134 | 1.00 | 38.08 |
| | HETATM | 4132 | O | HOH | 100 | -9.373 | 5.699 | -7.953 | 1.00 | 53.23 |
| | HETATM | 4133 | O | HOH | 101 | -10.137 | -0.553 | -6.742 | 1.00 | 47.72 |
| | HETATM | 4134 | O | HOH | 102 | 10.558 | -10.363 | 15.403 | 1.00 | 40.97 |

| | | | | | | | | | | |
|----|--------|------|---|-----|-----|---------|---------|---------|------|-------|
| 5 | HETATM | 4148 | O | HOH | 116 | 7.170 | 15.583 | 2.599 | 1.00 | 43.69 |
| | HETATM | 4149 | O | HOH | 117 | -1.966 | 10.606 | 3.572 | 1.00 | 52.63 |
| | HETATM | 4150 | O | HOH | 118 | 29.030 | 10.644 | 6.707 | 1.00 | 42.54 |
| | HETATM | 4151 | O | HOH | 119 | 0.468 | 4.354 | 8.374 | 1.00 | 38.69 |
| | HETATM | 4152 | O | HOH | 120 | 29.086 | 17.119 | 19.272 | 1.00 | 45.51 |
| 10 | HETATM | 4153 | O | HOH | 121 | 24.614 | 17.609 | 20.174 | 1.00 | 53.55 |
| | HETATM | 4154 | O | HOH | 122 | -15.318 | 0.362 | 26.686 | 1.00 | 36.77 |
| | HETATM | 4155 | O | HOH | 123 | -3.857 | -24.786 | 28.325 | 1.00 | 39.64 |
| | HETATM | 4156 | O | HOH | 124 | 21.728 | 22.178 | 31.983 | 1.00 | 43.73 |
| | HETATM | 4157 | O | HOH | 125 | 31.650 | -7.370 | 21.642 | 1.00 | 40.53 |
| 15 | HETATM | 4158 | O | HOH | 126 | 25.421 | 10.436 | 21.161 | 1.00 | 32.31 |
| | HETATM | 4159 | O | HOH | 127 | 10.317 | -9.457 | 12.998 | 1.00 | 37.77 |
| | HETATM | 4160 | O | HOH | 128 | 22.723 | 14.887 | 15.427 | 1.00 | 47.90 |
| | HETATM | 4161 | O | HOH | 129 | 6.702 | 9.556 | 37.596 | 1.00 | 47.81 |
| | HETATM | 4162 | O | HOH | 130 | 27.987 | 13.557 | 7.167 | 1.00 | 41.15 |
| 20 | HETATM | 4163 | O | HOH | 131 | 30.798 | 16.499 | 7.588 | 1.00 | 58.47 |
| | HETATM | 4164 | O | HOH | 132 | 10.071 | -0.571 | -20.393 | 1.00 | 38.79 |
| | HETATM | 4165 | O | HOH | 133 | 9.562 | 8.334 | -21.392 | 1.00 | 36.80 |
| | HETATM | 4166 | O | HOH | 134 | 6.712 | 6.058 | 8.822 | 1.00 | 37.43 |
| | HETATM | 4167 | O | HOH | 135 | 5.927 | 8.454 | 10.594 | 1.00 | 42.34 |
| 25 | HETATM | 4168 | O | HOH | 136 | 4.472 | 6.306 | 10.973 | 1.00 | 37.35 |
| | HETATM | 4169 | O | HOH | 137 | 6.792 | 7.721 | 7.051 | 1.00 | 47.23 |
| | HETATM | 4170 | O | HOH | 138 | 24.513 | 11.582 | 33.724 | 1.00 | 45.55 |
| | HETATM | 4171 | O | HOH | 139 | -2.528 | -20.361 | 12.354 | 1.00 | 52.13 |
| | HETATM | 4172 | O | HOH | 140 | -7.864 | 7.706 | 19.248 | 1.00 | 47.82 |
| 30 | HETATM | 4173 | O | HOH | 141 | 11.577 | -16.962 | 24.398 | 1.00 | 39.43 |
| | HETATM | 4174 | O | HOH | 142 | 18.087 | 12.263 | -5.507 | 1.00 | 33.36 |
| | HETATM | 4175 | O | HOH | 143 | -6.816 | -14.190 | 10.674 | 1.00 | 51.32 |
| | HETATM | 4176 | O | HOH | 144 | -7.377 | -16.701 | 33.528 | 1.00 | 57.11 |
| | HETATM | 4177 | O | HOH | 145 | -5.379 | -20.107 | 32.689 | 1.00 | 43.01 |
| 35 | HETATM | 4178 | O | HOH | 146 | 8.766 | -7.947 | -16.274 | 1.00 | 49.96 |
| | HETATM | 4179 | O | HOH | 147 | 10.946 | -7.937 | -18.142 | 1.00 | 55.67 |

END

5

Appendix 3

Atomic Coordinates for Human ER α Complexed With OHT

| | | | | | | | | | | | | |
|----|--------|----------|----------|----------|----------|--------|--------|--------|------|-------|---|----|
| 10 | CRYST1 | 58.242 | 58.242 | 277.467 | 90.00 | 90.00 | 120.00 | P | 65 | 2 | 2 | 12 |
| | ORIGX1 | 1.000000 | 0.000000 | 0.000000 | 0.000000 | | | | | | | |
| | ORIGX2 | 0.000000 | 1.000000 | 0.000000 | 0.000000 | | | | | | | |
| | ORIGX3 | 0.000000 | 0.000000 | 1.000000 | 0.000000 | | | | | | | |
| | SCALE1 | 0.017170 | 0.009913 | 0.000000 | 0.000000 | | | | | | | |
| 15 | SCALE2 | 0.000000 | 0.019826 | 0.000000 | 0.000000 | | | | | | | |
| | SCALE3 | 0.000000 | 0.000000 | 0.003604 | 0.000000 | | | | | | | |
| | ATOM | 1 | CB | LEU | 306 | 6.638 | 11.502 | 3.989 | 1.00 | 61.20 | | |
| | ATOM | 2 | C | LEU | 306 | 7.381 | 10.684 | 6.231 | 1.00 | 61.47 | | |
| 20 | ATOM | 3 | O | LEU | 306 | 6.407 | 11.020 | 6.905 | 1.00 | 62.09 | | |
| | ATOM | 4 | N | LEU | 306 | 6.369 | 9.128 | 4.588 | 1.00 | 62.32 | | |
| | ATOM | 5 | CA | LEU | 306 | 7.232 | 10.330 | 4.754 | 1.00 | 61.30 | | |
| | ATOM | 6 | N | ALA | 307 | 8.609 | 10.605 | 6.730 | 1.00 | 60.52 | | |
| | ATOM | 7 | CA | ALA | 307 | 8.891 | 10.912 | 8.125 | 1.00 | 58.77 | | |
| 25 | ATOM | 8 | CB | ALA | 307 | 10.318 | 10.501 | 8.465 | 1.00 | 59.70 | | |
| | ATOM | 9 | C | ALA | 307 | 8.692 | 12.393 | 8.429 | 1.00 | 57.51 | | |
| | ATOM | 10 | O | ALA | 307 | 8.451 | 12.770 | 9.574 | 1.00 | 57.64 | | |
| | ATOM | 11 | N | LEU | 308 | 8.789 | 13.228 | 7.400 | 1.00 | 55.82 | | |
| | ATOM | 12 | CA | LEU | 308 | 8.638 | 14.668 | 7.573 | 1.00 | 56.62 | | |
| 30 | ATOM | 13 | CB | LEU | 308 | 9.298 | 15.402 | 6.406 | 1.00 | 57.48 | | |
| | ATOM | 14 | CG | LEU | 308 | 10.637 | 14.822 | 5.948 | 1.00 | 59.17 | | |
| | ATOM | 15 | CD1 | LEU | 308 | 10.474 | 14.189 | 4.569 | 1.00 | 60.38 | | |
| | ATOM | 16 | CD2 | LEU | 308 | 11.694 | 15.920 | 5.933 | 1.00 | 58.46 | | |
| | ATOM | 17 | C | LEU | 308 | 7.190 | 15.130 | 7.710 | 1.00 | 56.51 | | |
| 35 | ATOM | 18 | O | LEU | 308 | 6.935 | 16.307 | 7.961 | 1.00 | 55.58 | | |
| | ATOM | 19 | N | SER | 309 | 6.246 | 14.208 | 7.546 | 1.00 | 57.04 | | |
| | ATOM | 20 | CA | SER | 309 | 4.828 | 14.544 | 7.657 | 1.00 | 56.46 | | |
| | ATOM | 21 | CB | SER | 309 | 4.034 | 13.896 | 6.514 | 1.00 | 56.79 | | |
| | ATOM | 22 | OG | SER | 309 | 4.071 | 12.479 | 6.588 | 1.00 | 57.23 | | |
| 40 | ATOM | 23 | C | SER | 309 | 4.261 | 14.095 | 9.003 | 1.00 | 56.13 | | |
| | ATOM | 24 | O | SER | 309 | 3.166 | 14.507 | 9.398 | 1.00 | 55.17 | | |
| | ATOM | 25 | N | LEU | 310 | 5.016 | 13.257 | 9.706 | 1.00 | 54.31 | | |
| | ATOM | 26 | CA | LEU | 310 | 4.591 | 12.749 | 11.004 | 1.00 | 53.55 | | |
| | ATOM | 27 | CB | LEU | 310 | 5.651 | 11.811 | 11.582 | 1.00 | 54.40 | | |
| 45 | ATOM | 28 | CG | LEU | 310 | 5.586 | 10.333 | 11.189 | 1.00 | 56.49 | | |
| | ATOM | 29 | CD1 | LEU | 310 | 5.530 | 10.200 | 9.676 | 1.00 | 57.06 | | |
| | ATOM | 30 | CD2 | LEU | 310 | 6.809 | 9.610 | 11.739 | 1.00 | 57.28 | | |
| | ATOM | 31 | C | LEU | 310 | 4.330 | 13.865 | 12.003 | 1.00 | 53.18 | | |
| | ATOM | 32 | O | LEU | 310 | 4.993 | 14.905 | 11.984 | 1.00 | 53.17 | | |
| 50 | ATOM | 33 | N | THR | 311 | 3.352 | 13.641 | 12.874 | 1.00 | 51.71 | | |
| | ATOM | 34 | CA | THR | 311 | 3.017 | 14.604 | 13.912 | 1.00 | 49.93 | | |
| | ATOM | 35 | CB | THR | 311 | 1.527 | 14.554 | 14.275 | 1.00 | 48.96 | | |
| | ATOM | 36 | OG1 | THR | 311 | 1.242 | 13.311 | 14.930 | 1.00 | 47.20 | | |
| | ATOM | 37 | CG2 | THR | 311 | 0.666 | 14.688 | 13.027 | 1.00 | 50.99 | | |
| 55 | ATOM | 38 | C | THR | 311 | 3.815 | 14.201 | 15.145 | 1.00 | 48.84 | | |
| | ATOM | 39 | O | THR | 311 | 4.371 | 13.103 | 15.197 | 1.00 | 46.66 | | |
| | ATOM | 40 | N | ALA | 312 | 3.857 | 15.078 | 16.141 | 1.00 | 48.76 | | |
| | ATOM | 41 | CA | ALA | 312 | 4.590 | 14.798 | 17.369 | 1.00 | 47.75 | | |
| | ATOM | 42 | CB | ALA | 312 | 4.359 | 15.910 | 18.378 | 1.00 | 47.06 | | |
| 60 | ATOM | 43 | C | ALA | 312 | 4.171 | 13.460 | 17.964 | 1.00 | 47.41 | | |

| | | | | | | | | | | |
|----|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 44 | O | ALA | 312 | 5.009 | 12.609 | 18.262 | 1.00 | 45.52 |
| | ATOM | 45 | N | ASP | 313 | 2.868 | 13.275 | 18.143 | 1.00 | 47.58 |
| | ATOM | 46 | CA | ASP | 313 | 2.367 | 12.032 | 18.714 | 1.00 | 47.63 |
| | ATOM | 47 | CB | ASP | 313 | 0.848 | 12.100 | 18.879 | 1.00 | 51.96 |
| | ATOM | 48 | CG | ASP | 313 | 0.430 | 12.872 | 20.118 | 1.00 | 56.21 |
| 10 | ATOM | 49 | OD1 | ASP | 313 | 1.314 | 13.234 | 20.929 | 1.00 | 56.38 |
| | ATOM | 50 | OD2 | ASP | 313 | -0.785 | 13.117 | 20.282 | 1.00 | 59.15 |
| | ATOM | 51 | C | ASP | 313 | 2.745 | 10.846 | 17.835 | 1.00 | 43.93 |
| | ATOM | 52 | O | ASP | 313 | 2.959 | 9.741 | 18.330 | 1.00 | 44.77 |
| | ATOM | 53 | N | GLN | 314 | 2.826 | 11.081 | 16.531 | 1.00 | 44.52 |
| 15 | ATOM | 54 | CA | GLN | 314 | 3.182 | 10.028 | 15.588 | 1.00 | 44.73 |
| | ATOM | 55 | CB | GLN | 314 | 2.849 | 10.464 | 14.156 | 1.00 | 45.05 |
| | ATOM | 56 | CG | GLN | 314 | 1.534 | 9.886 | 13.626 | 1.00 | 48.47 |
| | ATOM | 57 | CD | GLN | 314 | 0.982 | 10.646 | 12.428 | 1.00 | 50.37 |
| | ATOM | 58 | OE1 | GLN | 314 | 1.649 | 11.515 | 11.856 | 1.00 | 49.38 |
| 20 | ATOM | 59 | NE2 | GLN | 314 | -0.248 | 10.318 | 12.043 | 1.00 | 51.74 |
| | ATOM | 60 | C | GLN | 314 | 4.673 | 9.722 | 15.707 | 1.00 | 43.26 |
| | ATOM | 61 | O | GLN | 314 | 5.100 | 8.580 | 15.555 | 1.00 | 43.93 |
| | ATOM | 62 | N | MET | 315 | 5.459 | 10.757 | 15.980 | 1.00 | 42.29 |
| | ATOM | 63 | CA | MET | 315 | 6.901 | 10.606 | 16.130 | 1.00 | 41.26 |
| 25 | ATOM | 64 | CB | MET | 315 | 7.565 | 11.985 | 16.224 | 1.00 | 42.43 |
| | ATOM | 65 | CG | MET | 315 | 9.082 | 11.939 | 16.356 | 1.00 | 42.34 |
| | ATOM | 66 | SD | MET | 315 | 9.906 | 11.190 | 14.925 | 1.00 | 46.22 |
| | ATOM | 67 | CE | MET | 315 | 9.547 | 12.408 | 13.680 | 1.00 | 37.32 |
| | ATOM | 68 | C | MET | 315 | 7.218 | 9.791 | 17.379 | 1.00 | 38.89 |
| 30 | ATOM | 69 | O | MET | 315 | 8.002 | 8.841 | 17.335 | 1.00 | 40.02 |
| | ATOM | 70 | N | VAL | 316 | 6.599 | 10.165 | 18.491 | 1.00 | 37.65 |
| | ATOM | 71 | CA | VAL | 316 | 6.819 | 9.476 | 19.756 | 1.00 | 39.56 |
| | ATOM | 72 | CB | VAL | 316 | 6.023 | 10.136 | 20.897 | 1.00 | 39.22 |
| | ATOM | 73 | CG1 | VAL | 316 | 6.245 | 9.373 | 22.192 | 1.00 | 44.43 |
| 35 | ATOM | 74 | CG2 | VAL | 316 | 6.446 | 11.583 | 21.059 | 1.00 | 41.04 |
| | ATOM | 75 | C | VAL | 316 | 6.404 | 8.012 | 19.664 | 1.00 | 40.04 |
| | ATOM | 76 | O | VAL | 316 | 7.141 | 7.117 | 20.077 | 1.00 | 37.86 |
| | ATOM | 77 | N | SER | 317 | 5.215 | 7.767 | 19.127 | 1.00 | 41.90 |
| | ATOM | 78 | CA | SER | 317 | 4.733 | 6.400 | 18.997 | 1.00 | 41.68 |
| 40 | ATOM | 79 | CB | SER | 317 | 3.311 | 6.402 | 18.415 | 1.00 | 43.85 |
| | ATOM | 80 | OG | SER | 317 | 3.225 | 5.631 | 17.230 | 1.00 | 49.38 |
| | ATOM | 81 | C | SER | 317 | 5.696 | 5.601 | 18.114 | 1.00 | 39.72 |
| | ATOM | 82 | O | SER | 317 | 6.011 | 4.446 | 18.407 | 1.00 | 40.21 |
| | ATOM | 83 | N | ALA | 318 | 6.182 | 6.220 | 17.043 | 1.00 | 38.35 |
| 45 | ATOM | 84 | CA | ALA | 318 | 7.114 | 5.540 | 16.153 | 1.00 | 36.96 |
| | ATOM | 85 | CB | ALA | 318 | 7.485 | 6.448 | 14.986 | 1.00 | 37.92 |
| | ATOM | 86 | C | ALA | 318 | 8.375 | 5.137 | 16.920 | 1.00 | 38.31 |
| | ATOM | 87 | O | ALA | 318 | 8.820 | 3.992 | 16.844 | 1.00 | 33.94 |
| | ATOM | 88 | N | LEU | 319 | 8.938 | 6.089 | 17.664 | 1.00 | 36.92 |
| 50 | ATOM | 89 | CA | LEU | 319 | 10.161 | 5.854 | 18.438 | 1.00 | 38.56 |
| | ATOM | 90 | CB | LEU | 319 | 10.660 | 7.174 | 19.040 | 1.00 | 40.86 |
| | ATOM | 91 | CG | LEU | 319 | 11.136 | 8.264 | 18.071 | 1.00 | 41.25 |
| | ATOM | 92 | CD1 | LEU | 319 | 11.714 | 9.440 | 18.857 | 1.00 | 44.30 |
| | ATOM | 93 | CD2 | LEU | 319 | 12.182 | 7.693 | 17.140 | 1.00 | 42.61 |
| 55 | ATOM | 94 | C | LEU | 319 | 9.965 | 4.826 | 19.549 | 1.00 | 38.33 |
| | ATOM | 95 | O | LEU | 319 | 10.779 | 3.916 | 19.729 | 1.00 | 33.91 |
| | ATOM | 96 | N | LEU | 320 | 8.879 | 4.982 | 20.297 | 1.00 | 37.39 |
| | ATOM | 97 | CA | LEU | 320 | 8.567 | 4.067 | 21.387 | 1.00 | 41.55 |
| | ATOM | 98 | CB | LEU | 320 | 7.239 | 4.467 | 22.049 | 1.00 | 38.47 |
| 60 | ATOM | 99 | CG | LEU | 320 | 7.236 | 5.582 | 23.099 | 1.00 | 44.81 |
| | ATOM | 100 | CD1 | LEU | 320 | 5.876 | 5.634 | 23.802 | 1.00 | 44.96 |

| | | | | | | | | | | |
|----|------|-----|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 101 | CD2 | LEU | 320 | 8.334 | 5.332 | 24.112 | 1.00 | 43.36 |
| | ATOM | 102 | C | LEU | 320 | 8.466 | 2.642 | 20.843 | 1.00 | 41.11 |
| | ATOM | 103 | O | LEU | 320 | 8.971 | 1.697 | 21.443 | 1.00 | 41.87 |
| | ATOM | 104 | N | ASP | 321 | 7.812 | 2.504 | 19.696 | 1.00 | 43.94 |
| | ATOM | 105 | CA | ASP | 321 | 7.613 | 1.210 | 19.053 | 1.00 | 44.77 |
| 10 | ATOM | 106 | CB | ASP | 321 | 6.669 | 1.372 | 17.860 | 1.00 | 48.39 |
| | ATOM | 107 | CG | ASP | 321 | 5.206 | 1.318 | 18.255 | 1.00 | 52.39 |
| | ATOM | 108 | OD1 | ASP | 321 | 4.901 | 1.422 | 19.464 | 1.00 | 53.56 |
| | ATOM | 109 | OD2 | ASP | 321 | 4.357 | 1.172 | 17.346 | 1.00 | 55.81 |
| | ATOM | 110 | C | ASP | 321 | 8.911 | 0.565 | 18.568 | 1.00 | 44.37 |
| 15 | ATOM | 111 | O | ASP | 321 | 9.030 | -0.661 | 18.533 | 1.00 | 44.67 |
| | ATOM | 112 | N | ALA | 322 | 9.878 | 1.395 | 18.193 | 1.00 | 40.75 |
| | ATOM | 113 | CA | ALA | 322 | 11.153 | 0.905 | 17.686 | 1.00 | 37.81 |
| | ATOM | 114 | CB | ALA | 322 | 11.772 | 1.954 | 16.776 | 1.00 | 38.07 |
| | ATOM | 115 | C | ALA | 322 | 12.148 | 0.513 | 18.769 | 1.00 | 35.52 |
| 20 | ATOM | 116 | O | ALA | 322 | 13.219 | -0.020 | 18.473 | 1.00 | 36.11 |
| | ATOM | 117 | N | GLU | 323 | 11.799 | 0.768 | 20.022 | 1.00 | 35.61 |
| | ATOM | 118 | CA | GLU | 323 | 12.704 | 0.460 | 21.117 | 1.00 | 36.39 |
| | ATOM | 119 | CB | GLU | 323 | 12.042 | 0.768 | 22.459 | 1.00 | 35.09 |
| | ATOM | 120 | CG | GLU | 323 | 12.209 | 2.210 | 22.899 | 1.00 | 37.93 |
| 25 | ATOM | 121 | CD | GLU | 323 | 13.657 | 2.569 | 23.200 | 1.00 | 37.29 |
| | ATOM | 122 | OE1 | GLU | 323 | 14.313 | 3.173 | 22.326 | 1.00 | 34.21 |
| | ATOM | 123 | OE2 | GLU | 323 | 14.134 | 2.245 | 24.309 | 1.00 | 38.02 |
| | ATOM | 124 | C | GLU | 323 | 13.205 | -0.978 | 21.110 | 1.00 | 38.01 |
| | ATOM | 125 | O | GLU | 323 | 12.425 | -1.931 | 20.999 | 1.00 | 38.37 |
| 30 | ATOM | 126 | N | PRO | 324 | 14.527 | -1.151 | 21.225 | 1.00 | 36.03 |
| | ATOM | 127 | CD | PRO | 324 | 15.522 | -0.069 | 21.345 | 1.00 | 36.69 |
| | ATOM | 128 | CA | PRO | 324 | 15.158 | -2.474 | 21.240 | 1.00 | 36.42 |
| | ATOM | 129 | CB | PRO | 324 | 16.633 | -2.166 | 21.003 | 1.00 | 35.75 |
| | ATOM | 130 | CG | PRO | 324 | 16.811 | -0.807 | 21.610 | 1.00 | 35.46 |
| 35 | ATOM | 131 | C | PRO | 324 | 14.940 | -3.162 | 22.583 | 1.00 | 35.75 |
| | ATOM | 132 | O | PRO | 324 | 14.616 | -2.517 | 23.580 | 1.00 | 34.97 |
| | ATOM | 133 | N | PRO | 325 | 15.134 | -4.485 | 22.631 | 1.00 | 35.24 |
| | ATOM | 134 | CD | PRO | 325 | 15.530 | -5.386 | 21.534 | 1.00 | 37.02 |
| | ATOM | 135 | CA | PRO | 325 | 14.942 | -5.208 | 23.889 | 1.00 | 34.65 |
| 40 | ATOM | 136 | CB | PRO | 325 | 14.753 | -6.652 | 23.439 | 1.00 | 35.83 |
| | ATOM | 137 | CG | PRO | 325 | 15.589 | -6.743 | 22.200 | 1.00 | 34.88 |
| | ATOM | 138 | C | PRO | 325 | 16.132 | -5.070 | 24.824 | 1.00 | 34.51 |
| | ATOM | 139 | O | PRO | 325 | 17.237 | -4.723 | 24.399 | 1.00 | 29.92 |
| | ATOM | 140 | N | ILE | 326 | 15.899 | -5.322 | 26.106 | 1.00 | 33.62 |
| 45 | ATOM | 141 | CA | ILE | 326 | 16.975 | -5.265 | 27.075 | 1.00 | 35.02 |
| | ATOM | 142 | CB | ILE | 326 | 16.458 | -4.891 | 28.473 | 1.00 | 38.11 |
| | ATOM | 143 | CG2 | ILE | 326 | 17.557 | -5.110 | 29.504 | 1.00 | 38.70 |
| | ATOM | 144 | CG1 | ILE | 326 | 15.987 | -3.431 | 28.466 | 1.00 | 40.48 |
| | ATOM | 145 | CD1 | ILE | 326 | 16.035 | -2.747 | 29.815 | 1.00 | 42.96 |
| 50 | ATOM | 146 | C | ILE | 326 | 17.567 | -6.668 | 27.103 | 1.00 | 34.14 |
| | ATOM | 147 | O | ILE | 326 | 16.875 | -7.634 | 27.427 | 1.00 | 34.88 |
| | ATOM | 148 | N | LEU | 327 | 18.840 | -6.784 | 26.745 | 1.00 | 29.64 |
| | ATOM | 149 | CA | LEU | 327 | 19.493 | -8.083 | 26.716 | 1.00 | 29.54 |
| | ATOM | 150 | CB | LEU | 327 | 20.528 | -8.135 | 25.587 | 1.00 | 27.76 |
| 55 | ATOM | 151 | CG | LEU | 327 | 19.978 | -7.800 | 24.196 | 1.00 | 29.02 |
| | ATOM | 152 | CD1 | LEU | 327 | 21.068 | -7.993 | 23.139 | 1.00 | 28.76 |
| | ATOM | 153 | CD2 | LEU | 327 | 18.775 | -8.688 | 23.891 | 1.00 | 31.26 |
| | ATOM | 154 | C | LEU | 327 | 20.156 | -8.438 | 28.030 | 1.00 | 31.21 |
| | ATOM | 155 | O | LEU | 327 | 20.393 | -7.578 | 28.891 | 1.00 | 30.12 |
| 60 | ATOM | 156 | N | TYR | 328 | 20.445 | -9.725 | 28.181 | 1.00 | 30.99 |
| | ATOM | 157 | CA | TYR | 328 | 21.087 | -10.229 | 29.381 | 1.00 | 30.95 |

| | | | | | | | | | | |
|----|------|-----|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 158 | CB | TYR | 328 | 20.409 | -11.520 | 29.842 | 1.00 | 33.38 |
| | ATOM | 159 | CG | TYR | 328 | 19.194 | -11.272 | 30.686 | 1.00 | 33.05 |
| | ATOM | 160 | CD1 | TYR | 328 | 19.253 | -11.398 | 32.071 | 1.00 | 31.92 |
| | ATOM | 161 | CE1 | TYR | 328 | 18.152 | -11.114 | 32.864 | 1.00 | 36.01 |
| | ATOM | 162 | CD2 | TYR | 328 | 17.996 | -10.862 | 30.110 | 1.00 | 36.05 |
| 10 | ATOM | 163 | CE2 | TYR | 328 | 16.880 | -10.574 | 30.899 | 1.00 | 37.27 |
| | ATOM | 164 | CZ | TYR | 328 | 16.973 | -10.702 | 32.274 | 1.00 | 37.66 |
| | ATOM | 165 | OH | TYR | 328 | 15.896 | -10.397 | 33.071 | 1.00 | 44.66 |
| | ATOM | 166 | C | TYR | 328 | 22.529 | -10.520 | 29.067 | 1.00 | 33.66 |
| | ATOM | 167 | O | TYR | 328 | 22.884 | -10.744 | 27.910 | 1.00 | 34.78 |
| 15 | ATOM | 168 | N | SER | 329 | 23.359 | -10.496 | 30.103 | 1.00 | 33.97 |
| | ATOM | 169 | CA | SER | 329 | 24.767 | -10.800 | 29.962 | 1.00 | 37.29 |
| | ATOM | 170 | CB | SER | 329 | 25.526 | -10.342 | 31.204 | 1.00 | 36.51 |
| | ATOM | 171 | OG | SER | 329 | 26.787 | -10.965 | 31.282 | 1.00 | 37.13 |
| | ATOM | 172 | C | SER | 329 | 24.835 | -12.317 | 29.832 | 1.00 | 40.43 |
| 20 | ATOM | 173 | O | SER | 329 | 23.980 | -13.028 | 30.363 | 1.00 | 40.11 |
| | ATOM | 174 | N | GLU | 330 | 25.845 | -12.811 | 29.128 | 1.00 | 41.40 |
| | ATOM | 175 | CA | GLU | 330 | 25.992 | -14.242 | 28.928 | 1.00 | 47.43 |
| | ATOM | 176 | CB | GLU | 330 | 26.423 | -14.524 | 27.484 | 1.00 | 48.64 |
| | ATOM | 177 | CG | GLU | 330 | 25.278 | -14.870 | 26.542 | 1.00 | 50.20 |
| 25 | ATOM | 178 | CD | GLU | 330 | 25.765 | -15.405 | 25.198 | 1.00 | 53.25 |
| | ATOM | 179 | OE1 | GLU | 330 | 25.909 | -16.640 | 25.062 | 1.00 | 53.27 |
| | ATOM | 180 | OE2 | GLU | 330 | 26.004 | -14.590 | 24.280 | 1.00 | 51.80 |
| | ATOM | 181 | C | GLU | 330 | 26.999 | -14.852 | 29.893 | 1.00 | 49.67 |
| | ATOM | 182 | O | GLU | 330 | 28.207 | -14.741 | 29.696 | 1.00 | 50.11 |
| 30 | ATOM | 183 | N | TYR | 331 | 26.498 | -15.493 | 30.942 | 1.00 | 53.62 |
| | ATOM | 184 | CA | TYR | 331 | 27.373 | -16.130 | 31.921 | 1.00 | 58.16 |
| | ATOM | 185 | CB | TYR | 331 | 28.092 | -15.078 | 32.774 | 1.00 | 59.55 |
| | ATOM | 186 | CG | TYR | 331 | 27.239 | -14.460 | 33.860 | 1.00 | 63.08 |
| | ATOM | 187 | CD1 | TYR | 331 | 26.656 | -13.205 | 33.682 | 1.00 | 64.50 |
| 35 | ATOM | 188 | CE1 | TYR | 331 | 25.864 | -12.630 | 34.676 | 1.00 | 65.99 |
| | ATOM | 189 | CD2 | TYR | 331 | 27.010 | -15.128 | 35.065 | 1.00 | 63.52 |
| | ATOM | 190 | CE2 | TYR | 331 | 26.219 | -14.563 | 36.066 | 1.00 | 65.60 |
| | ATOM | 191 | CZ | TYR | 331 | 25.648 | -13.314 | 35.864 | 1.00 | 67.20 |
| | ATOM | 192 | OH | TYR | 331 | 24.855 | -12.753 | 36.839 | 1.00 | 67.40 |
| 40 | ATOM | 193 | C | TYR | 331 | 26.603 | -17.080 | 32.823 | 1.00 | 59.05 |
| | ATOM | 194 | O | TYR | 331 | 25.393 | -16.942 | 33.002 | 1.00 | 59.22 |
| | ATOM | 195 | N | ASP | 332 | 27.320 | -18.045 | 33.387 | 1.00 | 61.62 |
| | ATOM | 196 | CA | ASP | 332 | 26.719 | -19.026 | 34.281 | 1.00 | 64.20 |
| | ATOM | 197 | CB | ASP | 332 | 27.681 | -20.194 | 34.500 | 1.00 | 65.99 |
| 45 | ATOM | 198 | CG | ASP | 332 | 26.961 | -21.516 | 34.648 | 1.00 | 68.11 |
| | ATOM | 199 | OD1 | ASP | 332 | 27.575 | -22.564 | 34.351 | 1.00 | 69.54 |
| | ATOM | 200 | OD2 | ASP | 332 | 25.781 | -21.505 | 35.060 | 1.00 | 67.40 |
| | ATOM | 201 | C | ASP | 332 | 26.393 | -18.371 | 35.619 | 1.00 | 63.33 |
| | ATOM | 202 | O | ASP | 332 | 27.292 | -18.073 | 36.406 | 1.00 | 63.90 |
| 50 | ATOM | 203 | N | PRO | 333 | 25.096 | -18.148 | 35.896 | 1.00 | 63.64 |
| | ATOM | 204 | CD | PRO | 333 | 23.945 | -18.509 | 35.053 | 1.00 | 64.35 |
| | ATOM | 205 | CA | PRO | 333 | 24.677 | -17.521 | 37.154 | 1.00 | 63.52 |
| | ATOM | 206 | CB | PRO | 333 | 23.165 | -17.333 | 36.993 | 1.00 | 63.53 |
| | ATOM | 207 | CG | PRO | 333 | 22.866 | -17.611 | 35.556 | 1.00 | 64.15 |
| 55 | ATOM | 208 | C | PRO | 333 | 25.010 | -18.419 | 38.332 | 1.00 | 63.29 |
| | ATOM | 209 | O | PRO | 333 | 25.129 | -17.964 | 39.468 | 1.00 | 63.28 |
| | ATOM | 210 | N | THR | 334 | 25.160 | -19.704 | 38.037 | 1.00 | 64.26 |
| | ATOM | 211 | CA | THR | 334 | 25.475 | -20.697 | 39.050 | 1.00 | 66.09 |
| | ATOM | 212 | CB | THR | 334 | 24.929 | -22.080 | 38.645 | 1.00 | 66.90 |
| 60 | ATOM | 213 | OG1 | THR | 334 | 25.571 | -22.513 | 37.439 | 1.00 | 68.06 |
| | ATOM | 214 | CG2 | THR | 334 | 23.423 | -22.012 | 38.411 | 1.00 | 67.57 |

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|----|------|-----|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 215 | C | THR | 334 | 26.982 | -20.804 | 39.269 | 1.00 | 65.67 |
| | ATOM | 216 | O | THR | 334 | 27.432 | -21.323 | 40.289 | 1.00 | 64.77 |
| | ATOM | 217 | N | ARG | 335 | 27.759 | -20.308 | 38.313 | 1.00 | 65.65 |
| | ATOM | 218 | CA | ARG | 335 | 29.214 | -20.360 | 38.421 | 1.00 | 66.60 |
| | ATOM | 219 | CB | ARG | 335 | 29.835 | -20.500 | 37.030 | 1.00 | 66.74 |
| 10 | ATOM | 220 | C | ARG | 335 | 29.757 | -19.113 | 39.123 | 1.00 | 67.09 |
| | ATOM | 221 | O | ARG | 335 | 29.100 | -18.071 | 39.148 | 1.00 | 67.31 |
| | ATOM | 222 | N | PRO | 336 | 30.968 | -19.207 | 39.702 | 1.00 | 67.62 |
| | ATOM | 223 | CD | PRO | 336 | 31.820 | -20.408 | 39.713 | 1.00 | 67.30 |
| | ATOM | 224 | CA | PRO | 336 | 31.601 | -18.086 | 40.410 | 1.00 | 67.42 |
| 15 | ATOM | 225 | CB | PRO | 336 | 32.982 | -18.621 | 40.783 | 1.00 | 66.43 |
| | ATOM | 226 | CG | PRO | 336 | 32.829 | -20.097 | 40.779 | 1.00 | 67.52 |
| | ATOM | 227 | C | PRO | 336 | 31.701 | -16.828 | 39.561 | 1.00 | 68.26 |
| | ATOM | 228 | O | PRO | 336 | 31.996 | -16.895 | 38.371 | 1.00 | 69.04 |
| | ATOM | 229 | N | PHE | 337 | 31.460 | -15.681 | 40.183 | 1.00 | 69.49 |
| 20 | ATOM | 230 | CA | PHE | 337 | 31.529 | -14.408 | 39.480 | 1.00 | 71.39 |
| | ATOM | 231 | CB | PHE | 337 | 30.818 | -13.323 | 40.294 | 1.00 | 72.31 |
| | ATOM | 232 | CG | PHE | 337 | 31.219 | -11.924 | 39.921 | 1.00 | 73.21 |
| | ATOM | 233 | CD1 | PHE | 337 | 30.632 | -11.287 | 38.833 | 1.00 | 72.82 |
| | ATOM | 234 | CD2 | PHE | 337 | 32.191 | -11.245 | 40.653 | 1.00 | 73.43 |
| 25 | ATOM | 235 | CE1 | PHE | 337 | 31.006 | -9.993 | 38.479 | 1.00 | 73.28 |
| | ATOM | 236 | CE2 | PHE | 337 | 32.573 | -9.950 | 40.306 | 1.00 | 73.00 |
| | ATOM | 237 | CZ | PHE | 337 | 31.980 | -9.323 | 39.217 | 1.00 | 72.90 |
| | ATOM | 238 | C | PHE | 337 | 32.985 | -14.013 | 39.245 | 1.00 | 71.38 |
| | ATOM | 239 | O | PHE | 337 | 33.336 | -13.487 | 38.189 | 1.00 | 71.56 |
| 30 | ATOM | 240 | N | SER | 338 | 33.825 | -14.273 | 40.241 | 1.00 | 71.53 |
| | ATOM | 241 | CA | SER | 338 | 35.248 | -13.947 | 40.172 | 1.00 | 70.98 |
| | ATOM | 242 | CB | SER | 338 | 35.957 | -14.487 | 41.414 | 1.00 | 70.43 |
| | ATOM | 243 | OG | SER | 338 | 35.547 | -15.818 | 41.679 | 1.00 | 69.59 |
| | ATOM | 244 | C | SER | 338 | 35.931 | -14.504 | 38.924 | 1.00 | 71.20 |
| 35 | ATOM | 245 | O | SER | 338 | 36.951 | -13.972 | 38.475 | 1.00 | 71.35 |
| | ATOM | 246 | N | GLU | 339 | 35.368 | -15.573 | 38.369 | 1.00 | 70.20 |
| | ATOM | 247 | CA | GLU | 339 | 35.930 | -16.215 | 37.183 | 1.00 | 69.48 |
| | ATOM | 248 | CB | GLU | 339 | 35.279 | -17.585 | 36.971 | 1.00 | 71.07 |
| | ATOM | 249 | CG | GLU | 339 | 35.996 | -18.740 | 37.656 | 1.00 | 72.60 |
| 40 | ATOM | 250 | CD | GLU | 339 | 35.382 | -20.089 | 37.318 | 1.00 | 74.26 |
| | ATOM | 251 | OE1 | GLU | 339 | 34.786 | -20.220 | 36.227 | 1.00 | 73.51 |
| | ATOM | 252 | OE2 | GLU | 339 | 35.496 | -21.020 | 38.144 | 1.00 | 76.44 |
| | ATOM | 253 | C | GLU | 339 | 35.770 | -15.385 | 35.910 | 1.00 | 68.15 |
| | ATOM | 254 | O | GLU | 339 | 36.722 | -15.216 | 35.144 | 1.00 | 68.99 |
| 45 | ATOM | 255 | N | ALA | 340 | 34.562 | -14.874 | 35.694 | 1.00 | 64.41 |
| | ATOM | 256 | CA | ALA | 340 | 34.246 | -14.083 | 34.507 | 1.00 | 60.69 |
| | ATOM | 257 | CB | ALA | 340 | 32.767 | -13.709 | 34.523 | 1.00 | 61.17 |
| | ATOM | 258 | C | ALA | 340 | 35.096 | -12.824 | 34.326 | 1.00 | 57.00 |
| | ATOM | 259 | O | ALA | 340 | 35.634 | -12.270 | 35.287 | 1.00 | 57.46 |
| 50 | ATOM | 260 | N | SER | 341 | 35.215 | -12.388 | 33.076 | 1.00 | 52.15 |
| | ATOM | 261 | CA | SER | 341 | 35.972 | -11.188 | 32.736 | 1.00 | 46.53 |
| | ATOM | 262 | CB | SER | 341 | 36.839 | -11.439 | 31.497 | 1.00 | 48.64 |
| | ATOM | 263 | OG | SER | 341 | 37.184 | -10.226 | 30.846 | 1.00 | 46.48 |
| | ATOM | 264 | C | SER | 341 | 34.957 | -10.087 | 32.444 | 1.00 | 43.52 |
| 55 | ATOM | 265 | O | SER | 341 | 34.090 | -10.248 | 31.589 | 1.00 | 39.92 |
| | ATOM | 266 | N | MET | 342 | 35.052 | -8.978 | 33.166 | 1.00 | 41.24 |
| | ATOM | 267 | CA | MET | 342 | 34.121 | -7.875 | 32.960 | 1.00 | 42.46 |
| | ATOM | 268 | CB | MET | 342 | 34.449 | -6.723 | 33.912 | 1.00 | 45.61 |
| | ATOM | 269 | CG | MET | 342 | 33.228 | -6.089 | 34.560 | 1.00 | 52.39 |
| 60 | ATOM | 270 | SD | MET | 342 | 31.791 | -7.201 | 34.631 | 1.00 | 57.92 |
| | ATOM | 271 | CE | MET | 342 | 31.999 | -7.881 | 36.239 | 1.00 | 56.18 |

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|----|------|-----|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 272 | C | MET | 342 | 34.124 | -7.365 | 31.516 | 1.00 | 40.22 |
| | ATOM | 273 | O | MET | 342 | 33.063 | -7.121 | 30.938 | 1.00 | 39.23 |
| | ATOM | 274 | N | MET | 343 | 35.307 | -7.204 | 30.930 | 1.00 | 38.72 |
| | ATOM | 275 | CA | MET | 343 | 35.395 | -6.708 | 29.558 | 1.00 | 38.50 |
| | ATOM | 276 | CB | MET | 343 | 36.838 | -6.318 | 29.216 | 1.00 | 41.15 |
| 10 | ATOM | 277 | CG | MET | 343 | 37.022 | -5.749 | 27.804 | 1.00 | 40.31 |
| | ATOM | 278 | SD | MET | 343 | 36.032 | -4.260 | 27.427 | 1.00 | 45.23 |
| | ATOM | 279 | CE | MET | 343 | 36.113 | -3.358 | 28.987 | 1.00 | 40.45 |
| | ATOM | 280 | C | MET | 343 | 34.880 | -7.741 | 28.561 | 1.00 | 35.36 |
| | ATOM | 281 | O | MET | 343 | 34.368 | -7.384 | 27.501 | 1.00 | 35.51 |
| 15 | ATOM | 282 | N | GLY | 344 | 35.017 | -9.020 | 28.902 | 1.00 | 35.53 |
| | ATOM | 283 | CA | GLY | 344 | 34.533 | -10.072 | 28.024 | 1.00 | 33.41 |
| | ATOM | 284 | C | GLY | 344 | 33.015 | -10.063 | 28.047 | 1.00 | 31.74 |
| | ATOM | 285 | O | GLY | 344 | 32.359 | -10.233 | 27.019 | 1.00 | 29.58 |
| | ATOM | 286 | N | LEU | 345 | 32.459 | -9.860 | 29.238 | 1.00 | 32.89 |
| 20 | ATOM | 287 | CA | LEU | 345 | 31.011 | -9.804 | 29.415 | 1.00 | 34.95 |
| | ATOM | 288 | CB | LEU | 345 | 30.665 | -9.631 | 30.902 | 1.00 | 37.56 |
| | ATOM | 289 | CG | LEU | 345 | 30.942 | -10.774 | 31.883 | 1.00 | 43.03 |
| | ATOM | 290 | CD1 | LEU | 345 | 30.537 | -10.357 | 33.297 | 1.00 | 41.57 |
| | ATOM | 291 | CD2 | LEU | 345 | 30.164 | -11.998 | 31.449 | 1.00 | 42.80 |
| 25 | ATOM | 292 | C | LEU | 345 | 30.430 | -8.614 | 28.633 | 1.00 | 33.71 |
| | ATOM | 293 | O | LEU | 345 | 29.479 | -8.757 | 27.868 | 1.00 | 30.29 |
| | ATOM | 294 | N | LEU | 346 | 31.021 | -7.443 | 28.843 | 1.00 | 30.20 |
| | ATOM | 295 | CA | LEU | 346 | 30.569 | -6.217 | 28.193 | 1.00 | 32.00 |
| | ATOM | 296 | CB | LEU | 346 | 31.317 | -5.016 | 28.771 | 1.00 | 28.16 |
| 30 | ATOM | 297 | CG | LEU | 346 | 31.091 | -4.767 | 30.269 | 1.00 | 29.84 |
| | ATOM | 298 | CD1 | LEU | 346 | 31.815 | -3.498 | 30.668 | 1.00 | 29.98 |
| | ATOM | 299 | CD2 | LEU | 346 | 29.614 | -4.644 | 30.581 | 1.00 | 33.97 |
| | ATOM | 300 | C | LEU | 346 | 30.732 | -6.250 | 26.682 | 1.00 | 30.70 |
| | ATOM | 301 | O | LEU | 346 | 29.869 | -5.765 | 25.955 | 1.00 | 29.13 |
| 35 | ATOM | 302 | N | THR | 347 | 31.839 | -6.816 | 26.212 | 1.00 | 30.47 |
| | ATOM | 303 | CA | THR | 347 | 32.086 | -6.911 | 24.781 | 1.00 | 30.93 |
| | ATOM | 304 | CB | THR | 347 | 33.472 | -7.501 | 24.497 | 1.00 | 29.97 |
| | ATOM | 305 | OG1 | THR | 347 | 34.481 | -6.604 | 24.982 | 1.00 | 35.40 |
| | ATOM | 306 | CG2 | THR | 347 | 33.666 | -7.707 | 23.004 | 1.00 | 33.58 |
| 40 | ATOM | 307 | C | THR | 347 | 31.036 | -7.804 | 24.122 | 1.00 | 31.97 |
| | ATOM | 308 | O | THR | 347 | 30.516 | -7.486 | 23.049 | 1.00 | 30.75 |
| | ATOM | 309 | N | ASN | 348 | 30.737 | -8.926 | 24.768 | 1.00 | 29.31 |
| | ATOM | 310 | CA | ASN | 348 | 29.757 | -9.868 | 24.242 | 1.00 | 32.63 |
| | ATOM | 311 | CB | ASN | 348 | 29.767 | -11.161 | 25.065 | 1.00 | 31.64 |
| 45 | ATOM | 312 | CG | ASN | 348 | 28.646 | -12.117 | 24.662 | 1.00 | 39.14 |
| | ATOM | 313 | OD1 | ASN | 348 | 27.549 | -12.078 | 25.220 | 1.00 | 41.91 |
| | ATOM | 314 | ND2 | ASN | 348 | 28.920 | -12.970 | 23.683 | 1.00 | 42.05 |
| | ATOM | 315 | C | ASN | 348 | 28.361 | -9.251 | 24.262 | 1.00 | 29.02 |
| | ATOM | 316 | O | ASN | 348 | 27.558 | -9.477 | 23.353 | 1.00 | 32.76 |
| 50 | ATOM | 317 | N | LEU | 349 | 28.078 | -8.467 | 25.298 | 1.00 | 28.74 |
| | ATOM | 318 | CA | LEU | 349 | 26.782 | -7.811 | 25.421 | 1.00 | 28.58 |
| | ATOM | 319 | CB | LEU | 349 | 26.650 | -7.148 | 26.795 | 1.00 | 26.56 |
| | ATOM | 320 | CG | LEU | 349 | 25.376 | -6.328 | 27.050 | 1.00 | 33.67 |
| | ATOM | 321 | CD1 | LEU | 349 | 24.140 | -7.199 | 26.840 | 1.00 | 28.82 |
| 55 | ATOM | 322 | CD2 | LEU | 349 | 25.392 | -5.779 | 28.471 | 1.00 | 33.11 |
| | ATOM | 323 | C | LEU | 349 | 26.638 | -6.762 | 24.319 | 1.00 | 28.07 |
| | ATOM | 324 | O | LEU | 349 | 25.616 | -6.703 | 23.629 | 1.00 | 25.22 |
| | ATOM | 325 | N | ALA | 350 | 27.675 | -5.941 | 24.157 | 1.00 | 28.50 |
| | ATOM | 326 | CA | ALA | 350 | 27.668 | -4.886 | 23.148 | 1.00 | 28.46 |
| 60 | ATOM | 327 | CB | ALA | 350 | 28.972 | -4.094 | 23.209 | 1.00 | 28.12 |
| | ATOM | 328 | C | ALA | 350 | 27.468 | -5.461 | 21.750 | 1.00 | 28.75 |

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|----|------|-----|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 329 | O | ALA | 350 | 26.649 | -4.958 | 20.983 | 1.00 | 30.90 |
| | ATOM | 330 | N | ASP | 351 | 28.213 | -6.509 | 21.420 | 1.00 | 27.20 |
| | ATOM | 331 | CA | ASP | 351 | 28.093 | -7.143 | 20.112 | 1.00 | 29.75 |
| | ATOM | 332 | CB | ASP | 351 | 29.036 | -8.345 | 20.010 | 1.00 | 34.16 |
| | ATOM | 333 | CG | ASP | 351 | 30.498 | -7.940 | 19.978 | 1.00 | 37.50 |
| 10 | ATOM | 334 | OD1 | ASP | 351 | 31.354 | -8.831 | 20.148 | 1.00 | 37.55 |
| | ATOM | 335 | OD2 | ASP | 351 | 30.789 | -6.738 | 19.784 | 1.00 | 35.50 |
| | ATOM | 336 | C | ASP | 351 | 26.661 | -7.600 | 19.813 | 1.00 | 30.52 |
| | ATOM | 337 | O | ASP | 351 | 26.193 | -7.458 | 18.687 | 1.00 | 27.77 |
| | ATOM | 338 | N | ARG | 352 | 25.968 | -8.150 | 20.811 | 1.00 | 27.18 |
| 15 | ATOM | 339 | CA | ARG | 352 | 24.593 | -8.602 | 20.605 | 1.00 | 26.21 |
| | ATOM | 340 | CB | ARG | 352 | 24.148 | -9.534 | 21.752 | 1.00 | 26.52 |
| | ATOM | 341 | CG | ARG | 352 | 24.567 | -10.991 | 21.532 | 1.00 | 31.03 |
| | ATOM | 342 | CD | ARG | 352 | 24.128 | -11.911 | 22.666 | 1.00 | 29.80 |
| | ATOM | 343 | NE | ARG | 352 | 24.898 | -11.675 | 23.879 | 1.00 | 30.44 |
| 20 | ATOM | 344 | CZ | ARG | 352 | 24.364 | -11.363 | 25.054 | 1.00 | 31.68 |
| | ATOM | 345 | NH1 | ARG | 352 | 23.050 | -11.251 | 25.177 | 1.00 | 31.18 |
| | ATOM | 346 | NH2 | ARG | 352 | 25.144 | -11.148 | 26.104 | 1.00 | 32.03 |
| | ATOM | 347 | C | ARG | 352 | 23.642 | -7.411 | 20.502 | 1.00 | 27.16 |
| | ATOM | 348 | O | ARG | 352 | 22.702 | -7.426 | 19.708 | 1.00 | 26.65 |
| 25 | ATOM | 349 | N | GLU | 353 | 23.896 | -6.370 | 21.291 | 1.00 | 24.30 |
| | ATOM | 350 | CA | GLU | 353 | 23.045 | -5.178 | 21.261 | 1.00 | 26.39 |
| | ATOM | 351 | CB | GLU | 353 | 23.461 | -4.204 | 22.365 | 1.00 | 24.91 |
| | ATOM | 352 | CG | GLU | 353 | 23.147 | -4.669 | 23.771 | 1.00 | 27.93 |
| | ATOM | 353 | CD | GLU | 353 | 23.425 | -3.587 | 24.795 | 1.00 | 30.71 |
| 30 | ATOM | 354 | OE1 | GLU | 353 | 24.564 | -3.534 | 25.304 | 1.00 | 30.09 |
| | ATOM | 355 | OE2 | GLU | 353 | 22.506 | -2.789 | 25.085 | 1.00 | 30.53 |
| | ATOM | 356 | C | GLU | 353 | 23.131 | -4.456 | 19.920 | 1.00 | 24.27 |
| | ATOM | 357 | O | GLU | 353 | 22.169 | -3.826 | 19.467 | 1.00 | 28.71 |
| | ATOM | 358 | N | LEU | 354 | 24.296 | -4.540 | 19.293 | 1.00 | 26.61 |
| 35 | ATOM | 359 | CA | LEU | 354 | 24.522 | -3.872 | 18.017 | 1.00 | 26.62 |
| | ATOM | 360 | CB | LEU | 354 | 25.952 | -4.121 | 17.543 | 1.00 | 26.36 |
| | ATOM | 361 | CG | LEU | 354 | 26.372 | -3.257 | 16.351 | 1.00 | 29.24 |
| | ATOM | 362 | CD1 | LEU | 354 | 26.243 | -1.774 | 16.722 | 1.00 | 26.59 |
| | ATOM | 363 | CD2 | LEU | 354 | 27.794 | -3.607 | 15.962 | 1.00 | 28.88 |
| 40 | ATOM | 364 | C | LEU | 354 | 23.559 | -4.300 | 16.926 | 1.00 | 27.72 |
| | ATOM | 365 | O | LEU | 354 | 23.074 | -3.475 | 16.152 | 1.00 | 24.00 |
| | ATOM | 366 | N | VAL | 355 | 23.291 | -5.598 | 16.854 | 1.00 | 28.82 |
| | ATOM | 367 | CA | VAL | 355 | 22.386 | -6.125 | 15.844 | 1.00 | 29.45 |
| | ATOM | 368 | CB | VAL | 355 | 22.259 | -7.655 | 15.975 | 1.00 | 31.76 |
| 45 | ATOM | 369 | CG1 | VAL | 355 | 21.423 | -8.205 | 14.834 | 1.00 | 33.55 |
| | ATOM | 370 | CG2 | VAL | 355 | 23.649 | -8.282 | 15.998 | 1.00 | 31.36 |
| | ATOM | 371 | C | VAL | 355 | 21.020 | -5.499 | 16.035 | 1.00 | 27.71 |
| | ATOM | 372 | O | VAL | 355 | 20.382 | -5.039 | 15.080 | 1.00 | 29.61 |
| | ATOM | 373 | N | HIS | 356 | 20.580 | -5.473 | 17.288 | 1.00 | 27.76 |
| 50 | ATOM | 374 | CA | HIS | 356 | 19.291 | -4.906 | 17.627 | 1.00 | 28.35 |
| | ATOM | 375 | CB | HIS | 356 | 18.936 | -5.231 | 19.079 | 1.00 | 31.12 |
| | ATOM | 376 | CG | HIS | 356 | 18.602 | -6.675 | 19.307 | 1.00 | 35.93 |
| | ATOM | 377 | CD2 | HIS | 356 | 19.352 | -7.700 | 19.779 | 1.00 | 33.95 |
| | ATOM | 378 | ND1 | HIS | 356 | 17.363 | -7.208 | 19.018 | 1.00 | 36.62 |
| 55 | ATOM | 379 | CE1 | HIS | 356 | 17.364 | -8.499 | 19.304 | 1.00 | 33.33 |
| | ATOM | 380 | NE2 | HIS | 356 | 18.559 | -8.823 | 19.767 | 1.00 | 32.16 |
| | ATOM | 381 | C | HIS | 356 | 19.300 | -3.398 | 17.412 | 1.00 | 28.25 |
| | ATOM | 382 | O | HIS | 356 | 18.272 | -2.812 | 17.100 | 1.00 | 28.99 |
| | ATOM | 383 | N | MET | 357 | 20.457 | -2.765 | 17.574 | 1.00 | 25.31 |
| 60 | ATOM | 384 | CA | MET | 357 | 20.526 | -1.322 | 17.369 | 1.00 | 24.63 |
| | ATOM | 385 | CB | MET | 357 | 21.902 | -0.789 | 17.766 | 1.00 | 23.61 |

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|----|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 386 | CG | MET | 357 | 22.011 | 0.736 | 17.699 | 1.00 | 24.66 |
| | ATOM | 387 | SD | MET | 357 | 23.732 | 1.290 | 17.859 | 1.00 | 27.30 |
| | ATOM | 388 | CE | MET | 357 | 24.140 | 0.672 | 19.514 | 1.00 | 23.62 |
| | ATOM | 389 | C | MET | 357 | 20.256 | -1.011 | 15.898 | 1.00 | 24.83 |
| | ATOM | 390 | O | MET | 357 | 19.619 | -0.003 | 15.569 | 1.00 | 26.78 |
| 10 | ATOM | 391 | N | ILE | 358 | 20.757 | -1.874 | 15.020 | 1.00 | 26.25 |
| | ATOM | 392 | CA | ILE | 358 | 20.553 | -1.721 | 13.576 | 1.00 | 30.33 |
| | ATOM | 393 | CB | ILE | 358 | 21.204 | -2.888 | 12.789 | 1.00 | 33.86 |
| | ATOM | 394 | CG2 | ILE | 358 | 20.759 | -2.860 | 11.334 | 1.00 | 33.68 |
| | ATOM | 395 | CG1 | ILE | 358 | 22.728 | -2.799 | 12.874 | 1.00 | 36.89 |
| 15 | ATOM | 396 | CD1 | ILE | 358 | 23.299 | -1.469 | 12.451 | 1.00 | 39.10 |
| | ATOM | 397 | C | ILE | 358 | 19.055 | -1.721 | 13.310 | 1.00 | 32.20 |
| | ATOM | 398 | O | ILE | 358 | 18.519 | -0.817 | 12.662 | 1.00 | 32.02 |
| | ATOM | 399 | N | ASN | 359 | 18.379 | -2.748 | 13.814 | 1.00 | 33.12 |
| | ATOM | 400 | CA | ASN | 359 | 16.945 | -2.861 | 13.638 | 1.00 | 33.35 |
| 20 | ATOM | 401 | CB | ASN | 359 | 16.434 | -4.101 | 14.363 | 1.00 | 37.59 |
| | ATOM | 402 | CG | ASN | 359 | 16.739 | -5.374 | 13.627 | 1.00 | 44.38 |
| | ATOM | 403 | OD1 | ASN | 359 | 17.045 | -5.329 | 12.437 | 1.00 | 47.35 |
| | ATOM | 404 | ND2 | ASN | 359 | 16.673 | -6.508 | 14.320 | 1.00 | 42.48 |
| | ATOM | 405 | C | ASN | 359 | 16.224 | -1.634 | 14.149 | 1.00 | 32.74 |
| 25 | ATOM | 406 | O | ASN | 359 | 15.261 | -1.163 | 13.530 | 1.00 | 31.39 |
| | ATOM | 407 | N | TRP | 360 | 16.706 | -1.104 | 15.264 | 1.00 | 27.92 |
| | ATOM | 408 | CA | TRP | 360 | 16.102 | 0.087 | 15.842 | 1.00 | 29.47 |
| | ATOM | 409 | CB | TRP | 360 | 16.703 | 0.347 | 17.228 | 1.00 | 27.66 |
| | ATOM | 410 | CG | TRP | 360 | 16.522 | 1.747 | 17.707 | 1.00 | 30.40 |
| 30 | ATOM | 411 | CD2 | TRP | 360 | 17.493 | 2.801 | 17.657 | 1.00 | 27.54 |
| | ATOM | 412 | CE2 | TRP | 360 | 16.888 | 3.954 | 18.204 | 1.00 | 29.42 |
| | ATOM | 413 | CE3 | TRP | 360 | 18.819 | 2.883 | 17.205 | 1.00 | 28.37 |
| | ATOM | 414 | CD1 | TRP | 360 | 15.399 | 2.284 | 18.264 | 1.00 | 27.75 |
| | ATOM | 415 | NE1 | TRP | 360 | 15.609 | 3.611 | 18.566 | 1.00 | 30.84 |
| 35 | ATOM | 416 | CZ2 | TRP | 360 | 17.558 | 5.180 | 18.310 | 1.00 | 27.74 |
| | ATOM | 417 | CZ3 | TRP | 360 | 19.488 | 4.106 | 17.309 | 1.00 | 24.49 |
| | ATOM | 418 | CH2 | TRP | 360 | 18.853 | 5.232 | 17.858 | 1.00 | 25.09 |
| | ATOM | 419 | C | TRP | 360 | 16.312 | 1.296 | 14.926 | 1.00 | 27.90 |
| | ATOM | 420 | O | TRP | 360 | 15.360 | 2.002 | 14.581 | 1.00 | 28.83 |
| 40 | ATOM | 421 | N | ALA | 361 | 17.559 | 1.520 | 14.523 | 1.00 | 28.25 |
| | ATOM | 422 | CA | ALA | 361 | 17.894 | 2.637 | 13.645 | 1.00 | 29.20 |
| | ATOM | 423 | CB | ALA | 361 | 19.346 | 2.539 | 13.220 | 1.00 | 28.89 |
| | ATOM | 424 | C | ALA | 361 | 17.006 | 2.685 | 12.403 | 1.00 | 31.08 |
| | ATOM | 425 | O | ALA | 361 | 16.531 | 3.746 | 12.011 | 1.00 | 31.30 |
| 45 | ATOM | 426 | N | LYS | 362 | 16.795 | 1.526 | 11.783 | 1.00 | 30.93 |
| | ATOM | 427 | CA | LYS | 362 | 15.981 | 1.443 | 10.581 | 1.00 | 34.15 |
| | ATOM | 428 | CB | LYS | 362 | 16.012 | 0.016 | 10.023 | 1.00 | 33.67 |
| | ATOM | 429 | CG | LYS | 362 | 17.252 | -0.281 | 9.198 | 1.00 | 39.40 |
| | ATOM | 430 | CD | LYS | 362 | 17.547 | -1.774 | 9.136 | 1.00 | 43.60 |
| 50 | ATOM | 431 | CE | LYS | 362 | 18.852 | -2.046 | 8.389 | 1.00 | 47.06 |
| | ATOM | 432 | NZ | LYS | 362 | 19.178 | -3.507 | 8.288 | 1.00 | 50.34 |
| | ATOM | 433 | C | LYS | 362 | 14.545 | 1.872 | 10.815 | 1.00 | 35.81 |
| | ATOM | 434 | O | LYS | 362 | 13.821 | 2.168 | 9.859 | 1.00 | 37.95 |
| | ATOM | 435 | N | ARG | 363 | 14.134 | 1.921 | 12.079 | 1.00 | 34.23 |
| 55 | ATOM | 436 | CA | ARG | 363 | 12.770 | 2.313 | 12.409 | 1.00 | 36.04 |
| | ATOM | 437 | CB | ARG | 363 | 12.178 | 1.307 | 13.391 | 1.00 | 36.71 |
| | ATOM | 438 | CG | ARG | 363 | 12.169 | -0.110 | 12.827 | 1.00 | 40.36 |
| | ATOM | 439 | CD | ARG | 363 | 11.468 | -1.086 | 13.746 | 1.00 | 42.17 |
| | ATOM | 440 | NE | ARG | 363 | 10.161 | -0.586 | 14.158 | 1.00 | 45.19 |
| 60 | ATOM | 441 | CZ | ARG | 363 | 9.314 | -1.262 | 14.929 | 1.00 | 49.41 |
| | ATOM | 442 | NH1 | ARG | 363 | 9.642 | -2.467 | 15.374 | 1.00 | 48.02 |

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|----|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 443 | NH2 | ARG | 363 | 8.143 | -0.729 | 15.261 | 1.00 | 51.54 |
| | ATOM | 444 | C | ARG | 363 | 12.654 | 3.743 | 12.943 | 1.00 | 37.40 |
| | ATOM | 445 | O | ARG | 363 | 11.567 | 4.199 | 13.303 | 1.00 | 38.22 |
| | ATOM | 446 | N | VAL | 364 | 13.785 | 4.442 | 13.002 | 1.00 | 35.66 |
| | ATOM | 447 | CA | VAL | 364 | 13.804 | 5.836 | 13.431 | 1.00 | 34.06 |
| 10 | ATOM | 448 | CB | VAL | 364 | 15.231 | 6.271 | 13.827 | 1.00 | 33.87 |
| | ATOM | 449 | CG1 | VAL | 364 | 15.293 | 7.779 | 13.995 | 1.00 | 31.08 |
| | ATOM | 450 | CG2 | VAL | 364 | 15.641 | 5.571 | 15.113 | 1.00 | 31.30 |
| | ATOM | 451 | C | VAL | 364 | 13.360 | 6.591 | 12.171 | 1.00 | 33.19 |
| | ATOM | 452 | O | VAL | 364 | 14.028 | 6.531 | 11.146 | 1.00 | 33.04 |
| 15 | ATOM | 453 | N | PRO | 365 | 12.225 | 7.310 | 12.234 | 1.00 | 34.69 |
| | ATOM | 454 | CD | PRO | 365 | 11.359 | 7.492 | 13.413 | 1.00 | 34.19 |
| | ATOM | 455 | CA | PRO | 365 | 11.724 | 8.050 | 11.069 | 1.00 | 35.96 |
| | ATOM | 456 | CB | PRO | 365 | 10.608 | 8.918 | 11.645 | 1.00 | 36.59 |
| | ATOM | 457 | CG | PRO | 365 | 10.135 | 8.157 | 12.842 | 1.00 | 39.59 |
| 20 | ATOM | 458 | C | PRO | 365 | 12.756 | 8.878 | 10.321 | 1.00 | 37.19 |
| | ATOM | 459 | O | PRO | 365 | 13.430 | 9.726 | 10.907 | 1.00 | 40.29 |
| | ATOM | 460 | N | GLY | 366 | 12.878 | 8.624 | 9.023 | 1.00 | 34.78 |
| | ATOM | 461 | CA | GLY | 366 | 13.816 | 9.371 | 8.212 | 1.00 | 33.54 |
| | ATOM | 462 | C | GLY | 366 | 15.168 | 8.722 | 8.007 | 1.00 | 34.26 |
| 25 | ATOM | 463 | O | GLY | 366 | 15.858 | 9.035 | 7.034 | 1.00 | 37.15 |
| | ATOM | 464 | N | PHE | 367 | 15.554 | 7.814 | 8.901 | 1.00 | 33.13 |
| | ATOM | 465 | CA | PHE | 367 | 16.860 | 7.164 | 8.787 | 1.00 | 32.04 |
| | ATOM | 466 | CB | PHE | 367 | 17.138 | 6.291 | 10.016 | 1.00 | 30.22 |
| | ATOM | 467 | CG | PHE | 367 | 18.544 | 5.773 | 10.080 | 1.00 | 30.60 |
| 30 | ATOM | 468 | CD1 | PHE | 367 | 18.827 | 4.446 | 9.751 | 1.00 | 31.94 |
| | ATOM | 469 | CD2 | PHE | 367 | 19.589 | 6.601 | 10.485 | 1.00 | 29.20 |
| | ATOM | 470 | CE1 | PHE | 367 | 20.133 | 3.950 | 9.828 | 1.00 | 28.30 |
| | ATOM | 471 | CE2 | PHE | 367 | 20.896 | 6.122 | 10.568 | 1.00 | 28.12 |
| | ATOM | 472 | CZ | PHE | 367 | 21.171 | 4.791 | 10.240 | 1.00 | 25.41 |
| 35 | ATOM | 473 | C | PHE | 367 | 17.033 | 6.333 | 7.524 | 1.00 | 31.46 |
| | ATOM | 474 | O | PHE | 367 | 18.073 | 6.405 | 6.883 | 1.00 | 32.30 |
| | ATOM | 475 | N | VAL | 368 | 16.027 | 5.541 | 7.165 | 1.00 | 35.20 |
| | ATOM | 476 | CA | VAL | 368 | 16.123 | 4.718 | 5.959 | 1.00 | 38.98 |
| | ATOM | 477 | CB | VAL | 368 | 15.076 | 3.584 | 5.945 | 1.00 | 40.61 |
| 40 | ATOM | 478 | CG1 | VAL | 368 | 15.543 | 2.447 | 6.843 | 1.00 | 41.48 |
| | ATOM | 479 | CG2 | VAL | 368 | 13.717 | 4.113 | 6.390 | 1.00 | 41.60 |
| | ATOM | 480 | C | VAL | 368 | 15.965 | 5.523 | 4.673 | 1.00 | 40.06 |
| | ATOM | 481 | O | VAL | 368 | 16.156 | 4.992 | 3.579 | 1.00 | 41.66 |
| | ATOM | 482 | N | ASP | 369 | 15.608 | 6.798 | 4.798 | 1.00 | 38.65 |
| 45 | ATOM | 483 | CA | ASP | 369 | 15.465 | 7.646 | 3.621 | 1.00 | 37.15 |
| | ATOM | 484 | CB | ASP | 369 | 14.700 | 8.929 | 3.954 | 1.00 | 39.89 |
| | ATOM | 485 | CG | ASP | 369 | 13.254 | 8.671 | 4.302 | 1.00 | 45.59 |
| | ATOM | 486 | OD1 | ASP | 369 | 12.686 | 7.672 | 3.806 | 1.00 | 46.34 |
| | ATOM | 487 | OD2 | ASP | 369 | 12.681 | 9.472 | 5.074 | 1.00 | 49.13 |
| 50 | ATOM | 488 | C | ASP | 369 | 16.855 | 8.010 | 3.136 | 1.00 | 34.91 |
| | ATOM | 489 | O | ASP | 369 | 17.038 | 8.431 | 1.995 | 1.00 | 34.25 |
| | ATOM | 490 | N | LEU | 370 | 17.838 | 7.841 | 4.016 | 1.00 | 31.76 |
| | ATOM | 491 | CA | LEU | 370 | 19.229 | 8.153 | 3.705 | 1.00 | 28.08 |
| | ATOM | 492 | CB | LEU | 370 | 20.020 | 8.339 | 5.003 | 1.00 | 28.81 |
| 55 | ATOM | 493 | CG | LEU | 370 | 19.523 | 9.395 | 6.000 | 1.00 | 28.74 |
| | ATOM | 494 | CD1 | LEU | 370 | 20.315 | 9.275 | 7.299 | 1.00 | 30.81 |
| | ATOM | 495 | CD2 | LEU | 370 | 19.693 | 10.792 | 5.404 | 1.00 | 29.77 |
| | ATOM | 496 | C | LEU | 370 | 19.884 | 7.043 | 2.893 | 1.00 | 31.25 |
| | ATOM | 497 | O | LEU | 370 | 19.341 | 5.943 | 2.784 | 1.00 | 31.78 |
| 60 | ATOM | 498 | N | THR | 371 | 21.052 | 7.333 | 2.331 | 1.00 | 28.86 |
| | ATOM | 499 | CA | THR | 371 | 21.793 | 6.336 | 1.569 | 1.00 | 32.90 |

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|----|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 500 | CB | THR | 371 | 22.979 | 6.944 | 0.818 | 1.00 | 33.44 |
| | ATOM | 501 | OG1 | THR | 371 | 23.880 | 7.523 | 1.766 | 1.00 | 34.59 |
| | ATOM | 502 | CG2 | THR | 371 | 22.514 | 8.002 | -0.178 | 1.00 | 32.63 |
| | ATOM | 503 | C | THR | 371 | 22.373 | 5.315 | 2.539 | 1.00 | 35.31 |
| | ATOM | 504 | O | THR | 371 | 22.536 | 5.591 | 3.733 | 1.00 | 31.27 |
| 10 | ATOM | 505 | N | LEU | 372 | 22.702 | 4.141 | 2.015 | 1.00 | 34.34 |
| | ATOM | 506 | CA | LEU | 372 | 23.273 | 3.073 | 2.822 | 1.00 | 35.46 |
| | ATOM | 507 | CB | LEU | 372 | 23.518 | 1.841 | 1.944 | 1.00 | 37.73 |
| | ATOM | 508 | CG | LEU | 372 | 24.362 | 0.704 | 2.515 | 1.00 | 42.43 |
| | ATOM | 509 | CD1 | LEU | 372 | 23.690 | 0.145 | 3.757 | 1.00 | 45.60 |
| 15 | ATOM | 510 | CD2 | LEU | 372 | 24.534 | -0.383 | 1.455 | 1.00 | 44.29 |
| | ATOM | 511 | C | LEU | 372 | 24.587 | 3.548 | 3.444 | 1.00 | 36.95 |
| | ATOM | 512 | O | LEU | 372 | 24.813 | 3.374 | 4.643 | 1.00 | 35.57 |
| | ATOM | 513 | N | HIS | 373 | 25.442 | 4.159 | 2.627 | 1.00 | 35.68 |
| | ATOM | 514 | CA | HIS | 373 | 26.729 | 4.656 | 3.099 | 1.00 | 36.60 |
| 20 | ATOM | 515 | CB | HIS | 373 | 27.506 | 5.282 | 1.935 | 1.00 | 44.01 |
| | ATOM | 516 | CG | HIS | 373 | 28.538 | 6.280 | 2.360 | 1.00 | 50.69 |
| | ATOM | 517 | CD2 | HIS | 373 | 29.857 | 6.138 | 2.636 | 1.00 | 54.69 |
| | ATOM | 518 | ND1 | HIS | 373 | 28.246 | 7.613 | 2.561 | 1.00 | 53.77 |
| | ATOM | 519 | CE1 | HIS | 373 | 29.339 | 8.248 | 2.945 | 1.00 | 57.09 |
| 25 | ATOM | 520 | NE2 | HIS | 373 | 30.331 | 7.376 | 2.999 | 1.00 | 57.23 |
| | ATOM | 521 | C | HIS | 373 | 26.575 | 5.669 | 4.244 | 1.00 | 36.22 |
| | ATOM | 522 | O | HIS | 373 | 27.350 | 5.650 | 5.201 | 1.00 | 33.05 |
| | ATOM | 523 | N | ASP | 374 | 25.580 | 6.549 | 4.148 | 1.00 | 32.03 |
| | ATOM | 524 | CA | ASP | 374 | 25.342 | 7.541 | 5.196 | 1.00 | 30.76 |
| 30 | ATOM | 525 | CB | ASP | 374 | 24.354 | 8.603 | 4.713 | 1.00 | 30.12 |
| | ATOM | 526 | CG | ASP | 374 | 25.018 | 9.672 | 3.860 | 1.00 | 35.83 |
| | ATOM | 527 | OD1 | ASP | 374 | 26.264 | 9.744 | 3.842 | 1.00 | 34.39 |
| | ATOM | 528 | OD2 | ASP | 374 | 24.291 | 10.440 | 3.199 | 1.00 | 35.39 |
| | ATOM | 529 | C | ASP | 374 | 24.805 | 6.876 | 6.472 | 1.00 | 30.33 |
| 35 | ATOM | 530 | O | ASP | 374 | 25.152 | 7.275 | 7.587 | 1.00 | 27.04 |
| | ATOM | 531 | N | GLN | 375 | 23.944 | 5.877 | 6.309 | 1.00 | 25.71 |
| | ATOM | 532 | CA | GLN | 375 | 23.403 | 5.157 | 7.454 | 1.00 | 26.68 |
| | ATOM | 533 | CB | GLN | 375 | 22.424 | 4.077 | 6.993 | 1.00 | 29.70 |
| | ATOM | 534 | CG | GLN | 375 | 21.101 | 4.616 | 6.484 | 1.00 | 29.16 |
| 40 | ATOM | 535 | CD | GLN | 375 | 20.219 | 3.514 | 5.940 | 1.00 | 35.87 |
| | ATOM | 536 | OE1 | GLN | 375 | 20.155 | 2.426 | 6.510 | 1.00 | 30.97 |
| | ATOM | 537 | NE2 | GLN | 375 | 19.541 | 3.785 | 4.827 | 1.00 | 34.51 |
| | ATOM | 538 | C | GLN | 375 | 24.556 | 4.502 | 8.214 | 1.00 | 25.51 |
| | ATOM | 539 | O | GLN | 375 | 24.585 | 4.513 | 9.442 | 1.00 | 28.14 |
| 45 | ATOM | 540 | N | VAL | 376 | 25.504 | 3.938 | 7.475 | 1.00 | 26.62 |
| | ATOM | 541 | CA | VAL | 376 | 26.659 | 3.281 | 8.071 | 1.00 | 29.24 |
| | ATOM | 542 | CB | VAL | 376 | 27.531 | 2.597 | 7.003 | 1.00 | 29.66 |
| | ATOM | 543 | CG1 | VAL | 376 | 28.812 | 2.071 | 7.635 | 1.00 | 28.29 |
| | ATOM | 544 | CG2 | VAL | 376 | 26.745 | 1.469 | 6.341 | 1.00 | 29.90 |
| 50 | ATOM | 545 | C | VAL | 376 | 27.526 | 4.285 | 8.821 | 1.00 | 30.87 |
| | ATOM | 546 | O | VAL | 376 | 27.953 | 4.029 | 9.948 | 1.00 | 30.09 |
| | ATOM | 547 | N | HIS | 377 | 27.785 | 5.428 | 8.191 | 1.00 | 28.05 |
| | ATOM | 548 | CA | HIS | 377 | 28.602 | 6.457 | 8.814 | 1.00 | 28.68 |
| | ATOM | 549 | CB | HIS | 377 | 28.792 | 7.639 | 7.864 | 1.00 | 30.26 |
| 55 | ATOM | 550 | CG | HIS | 377 | 29.508 | 8.791 | 8.488 | 1.00 | 33.89 |
| | ATOM | 551 | CD2 | HIS | 377 | 29.073 | 10.017 | 8.863 | 1.00 | 34.99 |
| | ATOM | 552 | ND1 | HIS | 377 | 30.846 | 8.740 | 8.823 | 1.00 | 37.01 |
| | ATOM | 553 | CE1 | HIS | 377 | 31.201 | 9.884 | 9.377 | 1.00 | 34.79 |
| | ATOM | 554 | NE2 | HIS | 377 | 30.144 | 10.677 | 9.413 | 1.00 | 34.95 |
| 60 | ATOM | 555 | C | HIS | 377 | 27.983 | 6.954 | 10.114 | 1.00 | 25.13 |
| | ATOM | 556 | O | HIS | 377 | 28.677 | 7.102 | 11.115 | 1.00 | 25.93 |

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|----|------|-----|-----|------|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 557 | N | LEU | 378 | 26.678 | 7.206 | 10.107 | 1.00 | 24.58 |
| | ATOM | 558 | CA | LEU | 378 | 26.015 | 7.695 | 11.315 | 1.00 | 26.40 |
| | ATOM | 559 | CB | LEU | 378 | 24.542 | 8.001 | 11.027 | 1.00 | 26.29 |
| | ATOM | 560 | CG | LEU | 378 | 24.291 | 9.180 | 10.073 | 1.00 | 28.06 |
| | ATOM | 561 | CD1 | LEU | 378 | 22.778 | 9.353 | 9.869 | 1.00 | 27.66 |
| 10 | ATOM | 562 | CD2 | LEU | 378 | 24.911 | 10.458 | 10.642 | 1.00 | 30.08 |
| | ATOM | 563 | C | LEU | 378 | 26.120 | 6.695 | 12.459 | 1.00 | 28.55 |
| | ATOM | 564 | O | LEU | 378 | 26.379 | 7.075 | 13.605 | 1.00 | 24.76 |
| | ATOM | 565 | N | LEU | 379 | 25.919 | 5.414 | 12.153 | 1.00 | 24.29 |
| | ATOM | 566 | CA | LEU | 379 | 26.000 | 4.388 | 13.182 | 1.00 | 27.03 |
| 15 | ATOM | 567 | CB | LEU | 379 | 25.401 | 3.073 | 12.667 | 1.00 | 28.53 |
| | ATOM | 568 | CG | LEU | 379 | 23.875 | 3.023 | 12.845 | 1.00 | 30.29 |
| | ATOM | 569 | CD1 | LEU | 379 | 23.248 | 1.943 | 11.963 | 1.00 | 33.04 |
| | ATOM | 570 | CD2 | LEU | 379 | 23.563 | 2.759 | 14.312 | 1.00 | 29.45 |
| | ATOM | 571 | C | LEU | 379 | 27.430 | 4.176 | 13.670 | 1.00 | 27.18 |
| 20 | ATOM | 572 | O | LEU | 379 | 27.653 | 3.979 | 14.866 | 1.00 | 25.95 |
| | ATOM | 573 | N | GLU | 380 | 28.402 | 4.236 | 12.762 | 1.00 | 25.86 |
| | ATOM | 574 | CA | GLU | 380 | 29.786 | 4.054 | 13.173 | 1.00 | 27.58 |
| | ATOM | 575 | CB | GLU | 380 | 30.730 | 4.036 | 11.968 | 1.00 | 30.36 |
| | ATOM | 576 | CG | GLU | 380 | 32.172 | 3.785 | 12.380 | 1.00 | 37.98 |
| 25 | ATOM | 577 | CD | GLU | 380 | 33.080 | 3.471 | 11.210 | 1.00 | 45.23 |
| | ATOM | 578 | OE1 | GLU | 380 | 32.869 | 4.048 | 10.120 | 1.00 | 42.99 |
| | ATOM | 579 | OE2 | GLU | 380 | 34.004 | 2.646 | 11.386 | 1.00 | 45.79 |
| | ATOM | 580 | C | GLU | 380 | 30.218 | 5.159 | 14.133 | 1.00 | 27.50 |
| | ATOM | 581 | O | GLU | 380 | 31.056 | 4.937 | 15.010 | 1.00 | 26.67 |
| 30 | ATOM | 582 | N | ACYS | 381 | 29.637 | 6.339 | 13.965 | 0.75 | 24.89 |
| | ATOM | 583 | N | BCYS | 381 | 29.645 | 6.352 | 13.980 | 0.25 | 25.79 |
| | ATOM | 584 | CA | ACYS | 381 | 29.969 | 7.466 | 14.826 | 0.75 | 24.12 |
| | ATOM | 585 | CA | BCYS | 381 | 29.993 | 7.481 | 14.847 | 0.25 | 24.86 |
| | ATOM | 586 | CB | ACYS | 381 | 29.621 | 8.781 | 14.122 | 0.75 | 25.96 |
| 35 | ATOM | 587 | CB | BCYS | 381 | 29.766 | 8.814 | 14.115 | 0.25 | 25.62 |
| | ATOM | 588 | SG | ACYS | 381 | 30.698 | 9.192 | 12.732 | 0.75 | 31.63 |
| | ATOM | 589 | SG | BCYS | 381 | 30.227 | 10.312 | 15.059 | 0.25 | 25.40 |
| | ATOM | 590 | C | ACYS | 381 | 29.237 | 7.422 | 16.162 | 0.75 | 22.07 |
| | ATOM | 591 | C | BCYS | 381 | 29.211 | 7.498 | 16.159 | 0.25 | 23.97 |
| 40 | ATOM | 592 | O | ACYS | 381 | 29.812 | 7.730 | 17.206 | 0.75 | 21.97 |
| | ATOM | 593 | O | BCYS | 381 | 29.724 | 7.940 | 17.187 | 0.25 | 23.99 |
| | ATOM | 594 | N | ALA | 382 | 27.974 | 7.012 | 16.128 | 1.00 | 23.41 |
| | ATOM | 595 | CA | ALA | 382 | 27.140 | 7.015 | 17.318 | 1.00 | 22.83 |
| | ATOM | 596 | CB | ALA | 382 | 25.785 | 7.587 | 16.948 | 1.00 | 25.50 |
| 45 | ATOM | 597 | C | ALA | 382 | 26.913 | 5.755 | 18.131 | 1.00 | 25.39 |
| | ATOM | 598 | O | ALA | 382 | 26.374 | 5.837 | 19.234 | 1.00 | 23.09 |
| | ATOM | 599 | N | TRP | 383 | 27.311 | 4.602 | 17.615 | 1.00 | 25.98 |
| | ATOM | 600 | CA | TRP | 383 | 27.026 | 3.354 | 18.318 | 1.00 | 23.80 |
| | ATOM | 601 | CB | TRP | 383 | 27.669 | 2.172 | 17.580 | 1.00 | 22.52 |
| 50 | ATOM | 602 | CG | TRP | 383 | 29.130 | 2.054 | 17.762 | 1.00 | 24.42 |
| | ATOM | 603 | CD2 | TRP | 383 | 29.797 | 1.347 | 18.803 | 1.00 | 27.31 |
| | ATOM | 604 | CE2 | TRP | 383 | 31.182 | 1.484 | 18.579 | 1.00 | 28.24 |
| | ATOM | 605 | CE3 | TRP | 383 | 29.360 | 0.609 | 19.912 | 1.00 | 27.37 |
| | ATOM | 606 | CD1 | TRP | 383 | 30.102 | 2.578 | 16.965 | 1.00 | 24.58 |
| 55 | ATOM | 607 | NE1 | TRP | 383 | 31.342 | 2.239 | 17.446 | 1.00 | 27.35 |
| | ATOM | 608 | CZ2 | TRP | 383 | 32.133 | 0.909 | 19.420 | 1.00 | 28.76 |
| | ATOM | 609 | CZ3 | TRP | 383 | 30.305 | 0.039 | 20.745 | 1.00 | 28.09 |
| | ATOM | 610 | CH2 | TRP | 383 | 31.674 | 0.191 | 20.496 | 1.00 | 29.77 |
| | ATOM | 611 | C | TRP | 383 | 27.356 | 3.309 | 19.802 | 1.00 | 23.54 |
| 60 | ATOM | 612 | O | TRP | 383 | 26.526 | 2.866 | 20.584 | 1.00 | 22.90 |
| | ATOM | 613 | N | LEU | 384 | 28.542 | 3.765 | 20.211 | 1.00 | 20.37 |

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|----|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 614 | CA | LEU | 384 | 28.864 | 3.713 | 21.640 | 1.00 | 22.41 |
| | ATOM | 615 | CB | LEU | 384 | 30.369 | 3.890 | 21.883 | 1.00 | 24.98 |
| | ATOM | 616 | CG | LEU | 384 | 30.824 | 3.645 | 23.336 | 1.00 | 27.33 |
| | ATOM | 617 | CD1 | LEU | 384 | 30.273 | 2.305 | 23.853 | 1.00 | 29.71 |
| | ATOM | 618 | CD2 | LEU | 384 | 32.336 | 3.648 | 23.398 | 1.00 | 26.07 |
| 10 | ATOM | 619 | C | LEU | 384 | 28.075 | 4.732 | 22.453 | 1.00 | 19.44 |
| | ATOM | 620 | O | LEU | 384 | 27.706 | 4.458 | 23.595 | 1.00 | 23.24 |
| | ATOM | 621 | N | GLU | 385 | 27.807 | 5.909 | 21.885 | 1.00 | 20.80 |
| | ATOM | 622 | CA | GLU | 385 | 27.011 | 6.895 | 22.612 | 1.00 | 21.32 |
| | ATOM | 623 | CB | GLU | 385 | 26.861 | 8.177 | 21.797 | 1.00 | 21.91 |
| 15 | ATOM | 624 | CG | GLU | 385 | 28.115 | 9.020 | 21.705 | 1.00 | 21.61 |
| | ATOM | 625 | CD | GLU | 385 | 27.882 | 10.256 | 20.860 | 1.00 | 29.53 |
| | ATOM | 626 | OE1 | GLU | 385 | 27.374 | 11.256 | 21.401 | 1.00 | 30.54 |
| | ATOM | 627 | OE2 | GLU | 385 | 28.188 | 10.219 | 19.658 | 1.00 | 29.97 |
| | ATOM | 628 | C | GLU | 385 | 25.616 | 6.292 | 22.836 | 1.00 | 22.26 |
| 20 | ATOM | 629 | O | GLU | 385 | 25.022 | 6.438 | 23.902 | 1.00 | 22.26 |
| | ATOM | 630 | N | ILE | 386 | 25.101 | 5.617 | 21.812 | 1.00 | 22.03 |
| | ATOM | 631 | CA | ILE | 386 | 23.779 | 4.995 | 21.896 | 1.00 | 22.74 |
| | ATOM | 632 | CB | ILE | 386 | 23.328 | 4.455 | 20.498 | 1.00 | 22.88 |
| | ATOM | 633 | CG2 | ILE | 386 | 22.009 | 3.647 | 20.618 | 1.00 | 23.85 |
| 25 | ATOM | 634 | CG1 | ILE | 386 | 23.085 | 5.651 | 19.561 | 1.00 | 25.05 |
| | ATOM | 635 | CD1 | ILE | 386 | 22.994 | 5.297 | 18.078 | 1.00 | 26.42 |
| | ATOM | 636 | C | ILE | 386 | 23.766 | 3.897 | 22.961 | 1.00 | 22.50 |
| | ATOM | 637 | O | ILE | 386 | 22.823 | 3.818 | 23.746 | 1.00 | 24.75 |
| | ATOM | 638 | N | LEU | 387 | 24.810 | 3.071 | 23.020 | 1.00 | 22.25 |
| 30 | ATOM | 639 | CA | LEU | 387 | 24.868 | 2.030 | 24.051 | 1.00 | 22.95 |
| | ATOM | 640 | CB | LEU | 387 | 26.096 | 1.132 | 23.864 | 1.00 | 24.61 |
| | ATOM | 641 | CG | LEU | 387 | 26.070 | 0.194 | 22.654 | 1.00 | 23.21 |
| | ATOM | 642 | CD1 | LEU | 387 | 27.297 | -0.709 | 22.705 | 1.00 | 25.36 |
| | ATOM | 643 | CD2 | LEU | 387 | 24.791 | -0.631 | 22.652 | 1.00 | 26.29 |
| 35 | ATOM | 644 | C | LEU | 387 | 24.944 | 2.660 | 25.438 | 1.00 | 26.22 |
| | ATOM | 645 | O | LEU | 387 | 24.287 | 2.204 | 26.386 | 1.00 | 23.55 |
| | ATOM | 646 | N | MET | 388 | 25.751 | 3.713 | 25.554 | 1.00 | 23.92 |
| | ATOM | 647 | CA | MET | 388 | 25.924 | 4.385 | 26.835 | 1.00 | 24.26 |
| | ATOM | 648 | CB | MET | 388 | 27.088 | 5.378 | 26.761 | 1.00 | 23.87 |
| 40 | ATOM | 649 | CG | MET | 388 | 28.440 | 4.722 | 26.743 | 1.00 | 24.08 |
| | ATOM | 650 | SD | MET | 388 | 29.726 | 5.992 | 26.736 | 1.00 | 27.70 |
| | ATOM | 651 | CE | MET | 388 | 31.139 | 5.041 | 27.078 | 1.00 | 21.74 |
| | ATOM | 652 | C | MET | 388 | 24.660 | 5.094 | 27.321 | 1.00 | 23.33 |
| | ATOM | 653 | O | MET | 388 | 24.341 | 5.026 | 28.505 | 1.00 | 25.58 |
| 45 | ATOM | 654 | N | ILE | 389 | 23.935 | 5.775 | 26.436 | 1.00 | 24.62 |
| | ATOM | 655 | CA | ILE | 389 | 22.729 | 6.440 | 26.905 | 1.00 | 24.03 |
| | ATOM | 656 | CB | ILE | 389 | 22.132 | 7.439 | 25.852 | 1.00 | 27.01 |
| | ATOM | 657 | CG2 | ILE | 389 | 21.413 | 6.705 | 24.706 | 1.00 | 23.98 |
| | ATOM | 658 | CG1 | ILE | 389 | 21.185 | 8.402 | 26.584 | 1.00 | 25.49 |
| 50 | ATOM | 659 | CD1 | ILE | 389 | 20.431 | 9.383 | 25.683 | 1.00 | 25.45 |
| | ATOM | 660 | C | ILE | 389 | 21.694 | 5.401 | 27.349 | 1.00 | 26.54 |
| | ATOM | 661 | O | ILE | 389 | 20.938 | 5.631 | 28.294 | 1.00 | 22.58 |
| | ATOM | 662 | N | GLY | 390 | 21.679 | 4.247 | 26.687 | 1.00 | 27.14 |
| | ATOM | 663 | CA | GLY | 390 | 20.753 | 3.201 | 27.090 | 1.00 | 28.42 |
| 55 | ATOM | 664 | C | GLY | 390 | 21.133 | 2.719 | 28.482 | 1.00 | 29.67 |
| | ATOM | 665 | O | GLY | 390 | 20.275 | 2.521 | 29.348 | 1.00 | 29.21 |
| | ATOM | 666 | N | LEU | 391 | 22.433 | 2.547 | 28.699 | 1.00 | 26.06 |
| | ATOM | 667 | CA | LEU | 391 | 22.955 | 2.091 | 29.983 | 1.00 | 29.23 |
| | ATOM | 668 | CB | LEU | 391 | 24.476 | 1.937 | 29.899 | 1.00 | 28.37 |
| 60 | ATOM | 669 | CG | LEU | 391 | 25.206 | 1.656 | 31.210 | 1.00 | 30.81 |
| | ATOM | 670 | CD1 | LEU | 391 | 24.717 | 0.332 | 31.793 | 1.00 | 25.73 |

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|----|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 671 | CD2 | LEU | 391 | 26.709 | 1.619 | 30.958 | 1.00 | 25.25 |
| | ATOM | 672 | C | LEU | 391 | 22.603 | 3.070 | 31.104 | 1.00 | 30.84 |
| | ATOM | 673 | O | LEU | 391 | 22.156 | 2.669 | 32.186 | 1.00 | 29.19 |
| | ATOM | 674 | N | VAL | 392 | 22.817 | 4.355 | 30.850 | 1.00 | 28.91 |
| | ATOM | 675 | CA | VAL | 392 | 22.506 | 5.369 | 31.851 | 1.00 | 28.86 |
| 10 | ATOM | 676 | CB | VAL | 392 | 22.923 | 6.770 | 31.353 | 1.00 | 30.08 |
| | ATOM | 677 | CG1 | VAL | 392 | 22.329 | 7.854 | 32.237 | 1.00 | 32.32 |
| | ATOM | 678 | CG2 | VAL | 392 | 24.442 | 6.870 | 31.372 | 1.00 | 28.52 |
| | ATOM | 679 | C | VAL | 392 | 21.013 | 5.327 | 32.165 | 1.00 | 28.42 |
| | ATOM | 680 | O | VAL | 392 | 20.621 | 5.345 | 33.327 | 1.00 | 30.38 |
| 15 | ATOM | 681 | N | TRP | 393 | 20.191 | 5.241 | 31.125 | 1.00 | 28.23 |
| | ATOM | 682 | CA | TRP | 393 | 18.732 | 5.186 | 31.280 | 1.00 | 29.70 |
| | ATOM | 683 | CB | TRP | 393 | 18.066 | 5.046 | 29.906 | 1.00 | 30.09 |
| | ATOM | 684 | CG | TRP | 393 | 16.605 | 4.670 | 29.953 | 1.00 | 33.50 |
| | ATOM | 685 | CD2 | TRP | 393 | 15.516 | 5.499 | 30.369 | 1.00 | 31.76 |
| 20 | ATOM | 686 | CE2 | TRP | 393 | 14.336 | 4.725 | 30.264 | 1.00 | 38.11 |
| | ATOM | 687 | CE3 | TRP | 393 | 15.419 | 6.821 | 30.824 | 1.00 | 32.56 |
| | ATOM | 688 | CD1 | TRP | 393 | 16.057 | 3.459 | 29.618 | 1.00 | 34.31 |
| | ATOM | 689 | NE1 | TRP | 393 | 14.696 | 3.486 | 29.801 | 1.00 | 34.36 |
| | ATOM | 690 | CZ2 | TRP | 393 | 13.073 | 5.233 | 30.597 | 1.00 | 37.93 |
| 25 | ATOM | 691 | CZ3 | TRP | 393 | 14.162 | 7.326 | 31.155 | 1.00 | 35.24 |
| | ATOM | 692 | CH2 | TRP | 393 | 13.007 | 6.531 | 31.039 | 1.00 | 37.77 |
| | ATOM | 693 | C | TRP | 393 | 18.256 | 4.051 | 32.191 | 1.00 | 32.07 |
| | ATOM | 694 | O | TRP | 393 | 17.460 | 4.275 | 33.109 | 1.00 | 32.12 |
| | ATOM | 695 | N | ARG | 394 | 18.738 | 2.837 | 31.957 | 1.00 | 31.90 |
| 30 | ATOM | 696 | CA | ARG | 394 | 18.288 | 1.729 | 32.787 | 1.00 | 36.63 |
| | ATOM | 697 | CB | ARG | 394 | 18.492 | 0.389 | 32.065 | 1.00 | 36.41 |
| | ATOM | 698 | CG | ARG | 394 | 19.914 | 0.009 | 31.764 | 1.00 | 36.50 |
| | ATOM | 699 | CD | ARG | 394 | 19.929 | -1.132 | 30.748 | 1.00 | 36.34 |
| | ATOM | 700 | NE | ARG | 394 | 21.282 | -1.561 | 30.417 | 1.00 | 33.97 |
| 35 | ATOM | 701 | CZ | ARG | 394 | 21.864 | -1.350 | 29.239 | 1.00 | 31.61 |
| | ATOM | 702 | NH1 | ARG | 394 | 21.208 | -0.715 | 28.281 | 1.00 | 32.42 |
| | ATOM | 703 | NH2 | ARG | 394 | 23.098 | -1.784 | 29.022 | 1.00 | 29.81 |
| | ATOM | 704 | C | ARG | 394 | 18.911 | 1.697 | 34.180 | 1.00 | 36.69 |
| | ATOM | 705 | O | ARG | 394 | 18.445 | 0.966 | 35.048 | 1.00 | 37.07 |
| 40 | ATOM | 706 | N | SER | 395 | 19.954 | 2.492 | 34.395 | 1.00 | 33.63 |
| | ATOM | 707 | CA | SER | 395 | 20.603 | 2.564 | 35.701 | 1.00 | 35.69 |
| | ATOM | 708 | CB | SER | 395 | 22.112 | 2.784 | 35.540 | 1.00 | 32.94 |
| | ATOM | 709 | OG | SER | 395 | 22.696 | 1.811 | 34.688 | 1.00 | 32.37 |
| | ATOM | 710 | C | SER | 395 | 20.010 | 3.713 | 36.531 | 1.00 | 36.44 |
| 45 | ATOM | 711 | O | SER | 395 | 20.389 | 3.916 | 37.687 | 1.00 | 38.68 |
| | ATOM | 712 | N | MET | 396 | 19.076 | 4.449 | 35.937 | 1.00 | 36.46 |
| | ATOM | 713 | CA | MET | 396 | 18.431 | 5.588 | 36.589 | 1.00 | 43.08 |
| | ATOM | 714 | CB | MET | 396 | 17.275 | 6.104 | 35.725 | 1.00 | 43.87 |
| | ATOM | 715 | CG | MET | 396 | 17.481 | 7.507 | 35.176 | 1.00 | 46.18 |
| 50 | ATOM | 716 | SD | MET | 396 | 15.962 | 8.278 | 34.581 | 1.00 | 49.58 |
| | ATOM | 717 | CE | MET | 396 | 14.988 | 8.298 | 36.065 | 1.00 | 53.58 |
| | ATOM | 718 | C | MET | 396 | 17.906 | 5.303 | 37.992 | 1.00 | 46.18 |
| | ATOM | 719 | O | MET | 396 | 18.125 | 6.089 | 38.913 | 1.00 | 46.34 |
| | ATOM | 720 | N | GLU | 397 | 17.215 | 4.180 | 38.152 | 1.00 | 49.39 |
| 55 | ATOM | 721 | CA | GLU | 397 | 16.645 | 3.821 | 39.444 | 1.00 | 52.12 |
| | ATOM | 722 | CB | GLU | 397 | 15.296 | 3.130 | 39.246 | 1.00 | 55.34 |
| | ATOM | 723 | CG | GLU | 397 | 14.166 | 4.073 | 38.873 | 1.00 | 58.86 |
| | ATOM | 724 | CD | GLU | 397 | 13.195 | 3.448 | 37.891 | 1.00 | 63.28 |
| | ATOM | 725 | OE1 | GLU | 397 | 13.660 | 2.925 | 36.854 | 1.00 | 64.68 |
| 60 | ATOM | 726 | OE2 | GLU | 397 | 11.972 | 3.475 | 38.155 | 1.00 | 65.39 |
| | ATOM | 727 | C | GLU | 397 | 17.548 | 2.933 | 40.283 | 1.00 | 52.75 |

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|----|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 728 | O | GLU | 397 | 17.071 | 2.187 | 41.139 | 1.00 | 53.96 |
| | ATOM | 729 | N | HIS | 398 | 18.851 | 3.014 | 40.040 | 1.00 | 50.25 |
| | ATOM | 730 | CA | HIS | 398 | 19.813 | 2.220 | 40.792 | 1.00 | 49.34 |
| | ATOM | 731 | CB | HIS | 398 | 20.271 | 1.018 | 39.963 | 1.00 | 52.04 |
| | ATOM | 732 | CG | HIS | 398 | 19.187 | 0.017 | 39.721 | 1.00 | 53.95 |
| 10 | ATOM | 733 | CD2 | HIS | 398 | 18.750 | -1.022 | 40.472 | 1.00 | 53.92 |
| | ATOM | 734 | ND1 | HIS | 398 | 18.374 | 0.054 | 38.608 | 1.00 | 55.91 |
| | ATOM | 735 | CE1 | HIS | 398 | 17.482 | -0.917 | 38.685 | 1.00 | 55.53 |
| | ATOM | 736 | NE2 | HIS | 398 | 17.688 | -1.585 | 39.806 | 1.00 | 55.81 |
| | ATOM | 737 | C | HIS | 398 | 20.999 | 3.084 | 41.196 | 1.00 | 47.44 |
| 15 | ATOM | 738 | O | HIS | 398 | 22.121 | 2.887 | 40.730 | 1.00 | 44.91 |
| | ATOM | 739 | N | PRO | 399 | 20.755 | 4.049 | 42.096 | 1.00 | 46.45 |
| | ATOM | 740 | CD | PRO | 399 | 19.443 | 4.300 | 42.721 | 1.00 | 47.27 |
| | ATOM | 741 | CA | PRO | 399 | 21.785 | 4.968 | 42.586 | 1.00 | 45.35 |
| | ATOM | 742 | CB | PRO | 399 | 21.127 | 5.631 | 43.793 | 1.00 | 47.40 |
| 20 | ATOM | 743 | CG | PRO | 399 | 19.660 | 5.561 | 43.504 | 1.00 | 47.72 |
| | ATOM | 744 | C | PRO | 399 | 23.086 | 4.270 | 42.958 | 1.00 | 44.70 |
| | ATOM | 745 | O | PRO | 399 | 23.078 | 3.233 | 43.627 | 1.00 | 46.46 |
| | ATOM | 746 | N | GLY | 400 | 24.202 | 4.840 | 42.509 | 1.00 | 41.57 |
| | ATOM | 747 | CA | GLY | 400 | 25.506 | 4.281 | 42.813 | 1.00 | 39.84 |
| 25 | ATOM | 748 | C | GLY | 400 | 25.907 | 3.047 | 42.022 | 1.00 | 37.85 |
| | ATOM | 749 | O | GLY | 400 | 27.027 | 2.560 | 42.176 | 1.00 | 40.48 |
| | ATOM | 750 | N | LYS | 401 | 25.012 | 2.537 | 41.180 | 1.00 | 36.39 |
| | ATOM | 751 | CA | LYS | 401 | 25.315 | 1.344 | 40.390 | 1.00 | 34.47 |
| | ATOM | 752 | CB | LYS | 401 | 24.562 | 0.130 | 40.947 | 1.00 | 36.12 |
| 30 | ATOM | 753 | CG | LYS | 401 | 24.633 | -0.007 | 42.466 | 1.00 | 39.30 |
| | ATOM | 754 | CD | LYS | 401 | 24.288 | -1.429 | 42.903 | 1.00 | 44.38 |
| | ATOM | 755 | CE | LYS | 401 | 24.459 | -1.605 | 44.408 | 1.00 | 46.68 |
| | ATOM | 756 | NZ | LYS | 401 | 24.968 | -2.969 | 44.747 | 1.00 | 53.37 |
| | ATOM | 757 | C | LYS | 401 | 24.969 | 1.485 | 38.911 | 1.00 | 32.34 |
| 35 | ATOM | 758 | O | LYS | 401 | 24.141 | 2.308 | 38.531 | 1.00 | 31.16 |
| | ATOM | 759 | N | LEU | 402 | 25.612 | 0.663 | 38.086 | 1.00 | 28.52 |
| | ATOM | 760 | CA | LEU | 402 | 25.358 | 0.658 | 36.648 | 1.00 | 29.06 |
| | ATOM | 761 | CB | LEU | 402 | 26.661 | 0.847 | 35.867 | 1.00 | 29.26 |
| | ATOM | 762 | CG | LEU | 402 | 27.278 | 2.242 | 36.029 | 1.00 | 24.67 |
| 40 | ATOM | 763 | CD1 | LEU | 402 | 28.623 | 2.310 | 35.310 | 1.00 | 27.47 |
| | ATOM | 764 | CD2 | LEU | 402 | 26.312 | 3.277 | 35.482 | 1.00 | 24.93 |
| | ATOM | 765 | C | LEU | 402 | 24.755 | -0.686 | 36.292 | 1.00 | 30.43 |
| | ATOM | 766 | O | LEU | 402 | 25.367 | -1.727 | 36.535 | 1.00 | 31.36 |
| | ATOM | 767 | N | LEU | 403 | 23.552 | -0.658 | 35.735 | 1.00 | 31.07 |
| 45 | ATOM | 768 | CA | LEU | 403 | 22.873 | -1.880 | 35.335 | 1.00 | 32.96 |
| | ATOM | 769 | CB | LEU | 403 | 21.361 | -1.693 | 35.434 | 1.00 | 33.86 |
| | ATOM | 770 | CG | LEU | 403 | 20.551 | -2.991 | 35.415 | 1.00 | 39.29 |
| | ATOM | 771 | CD1 | LEU | 403 | 20.584 | -3.637 | 36.806 | 1.00 | 43.62 |
| | ATOM | 772 | CD2 | LEU | 403 | 19.128 | -2.689 | 34.998 | 1.00 | 41.32 |
| 50 | ATOM | 773 | C | LEU | 403 | 23.255 | -2.218 | 33.899 | 1.00 | 30.06 |
| | ATOM | 774 | O | LEU | 403 | 22.543 | -1.870 | 32.956 | 1.00 | 31.63 |
| | ATOM | 775 | N | PHE | 404 | 24.383 | -2.893 | 33.733 | 1.00 | 29.19 |
| | ATOM | 776 | CA | PHE | 404 | 24.834 | -3.256 | 32.403 | 1.00 | 28.93 |
| | ATOM | 777 | CB | PHE | 404 | 26.201 | -3.929 | 32.493 | 1.00 | 30.05 |
| 55 | ATOM | 778 | CG | PHE | 404 | 27.305 | -2.998 | 32.926 | 1.00 | 30.78 |
| | ATOM | 779 | CD1 | PHE | 404 | 27.794 | -3.033 | 34.228 | 1.00 | 32.91 |
| | ATOM | 780 | CD2 | PHE | 404 | 27.848 | -2.078 | 32.030 | 1.00 | 32.75 |
| | ATOM | 781 | CE1 | PHE | 404 | 28.816 | -2.160 | 34.638 | 1.00 | 34.73 |
| | ATOM | 782 | CE2 | PHE | 404 | 28.864 | -1.205 | 32.423 | 1.00 | 30.68 |
| 60 | ATOM | 783 | CZ | PHE | 404 | 29.350 | -1.242 | 33.727 | 1.00 | 31.43 |
| | ATOM | 784 | C | PHE | 404 | 23.809 | -4.181 | 31.756 | 1.00 | 30.80 |

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|----|------|-----|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 785 | O | PHE | 404 | 23.625 | -4.175 | 30.538 | 1.00 | 28.09 |
| | ATOM | 786 | N | ALA | 405 | 23.138 | -4.967 | 32.594 | 1.00 | 30.25 |
| | ATOM | 787 | CA | ALA | 405 | 22.104 | -5.910 | 32.163 | 1.00 | 29.78 |
| | ATOM | 788 | CB | ALA | 405 | 22.745 | -7.172 | 31.598 | 1.00 | 29.97 |
| | ATOM | 789 | C | ALA | 405 | 21.309 | -6.237 | 33.429 | 1.00 | 31.95 |
| 10 | ATOM | 790 | O | ALA | 405 | 21.785 | -5.995 | 34.535 | 1.00 | 32.36 |
| | ATOM | 791 | N | PRO | 406 | 20.088 | -6.779 | 33.288 | 1.00 | 34.40 |
| | ATOM | 792 | CD | PRO | 406 | 19.356 | -7.102 | 32.053 | 1.00 | 35.81 |
| | ATOM | 793 | CA | PRO | 406 | 19.303 | -7.101 | 34.490 | 1.00 | 36.41 |
| | ATOM | 794 | CB | PRO | 406 | 17.985 | -7.654 | 33.935 | 1.00 | 35.38 |
| 15 | ATOM | 795 | CG | PRO | 406 | 17.922 | -7.153 | 32.519 | 1.00 | 36.49 |
| | ATOM | 796 | C | PRO | 406 | 19.997 | -8.084 | 35.433 | 1.00 | 37.32 |
| | ATOM | 797 | O | PRO | 406 | 19.698 | -8.112 | 36.626 | 1.00 | 38.34 |
| | ATOM | 798 | N | ASN | 407 | 20.924 | -8.877 | 34.902 | 1.00 | 36.69 |
| | ATOM | 799 | CA | ASN | 407 | 21.652 | -9.847 | 35.712 | 1.00 | 38.85 |
| 20 | ATOM | 800 | CB | ASN | 407 | 21.582 | -11.243 | 35.083 | 1.00 | 39.69 |
| | ATOM | 801 | CG | ASN | 407 | 22.232 | -11.306 | 33.711 | 1.00 | 44.10 |
| | ATOM | 802 | OD1 | ASN | 407 | 22.345 | -10.296 | 33.009 | 1.00 | 37.78 |
| | ATOM | 803 | ND2 | ASN | 407 | 22.660 | -12.503 | 33.319 | 1.00 | 45.74 |
| | ATOM | 804 | C | ASN | 407 | 23.100 | -9.435 | 35.874 | 1.00 | 38.12 |
| 25 | ATOM | 805 | O | ASN | 407 | 23.965 | -10.256 | 36.178 | 1.00 | 39.81 |
| | ATOM | 806 | N | LEU | 408 | 23.364 | -8.149 | 35.671 | 1.00 | 37.80 |
| | ATOM | 807 | CA | LEU | 408 | 24.713 | -7.631 | 35.799 | 1.00 | 36.89 |
| | ATOM | 808 | CB | LEU | 408 | 25.449 | -7.720 | 34.459 | 1.00 | 36.09 |
| | ATOM | 809 | CG | LEU | 408 | 26.972 | -7.609 | 34.550 | 1.00 | 35.08 |
| 30 | ATOM | 810 | CD1 | LEU | 408 | 27.525 | -8.775 | 35.354 | 1.00 | 39.15 |
| | ATOM | 811 | CD2 | LEU | 408 | 27.578 | -7.587 | 33.158 | 1.00 | 36.85 |
| | ATOM | 812 | C | LEU | 408 | 24.670 | -6.187 | 36.286 | 1.00 | 40.55 |
| | ATOM | 813 | O | LEU | 408 | 24.646 | -5.248 | 35.491 | 1.00 | 38.29 |
| | ATOM | 814 | N | LEU | 409 | 24.644 | -6.034 | 37.607 | 1.00 | 39.50 |
| 35 | ATOM | 815 | CA | LEU | 409 | 24.606 | -4.733 | 38.257 | 1.00 | 41.00 |
| | ATOM | 816 | CB | LEU | 409 | 23.392 | -4.658 | 39.184 | 1.00 | 43.69 |
| | ATOM | 817 | CG | LEU | 409 | 23.164 | -3.382 | 39.993 | 1.00 | 47.35 |
| | ATOM | 818 | CD1 | LEU | 409 | 22.848 | -2.233 | 39.058 | 1.00 | 47.09 |
| | ATOM | 819 | CD2 | LEU | 409 | 22.014 | -3.603 | 40.976 | 1.00 | 49.38 |
| 40 | ATOM | 820 | C | LEU | 409 | 25.894 | -4.566 | 39.060 | 1.00 | 41.80 |
| | ATOM | 821 | O | LEU | 409 | 26.178 | -5.358 | 39.960 | 1.00 | 41.00 |
| | ATOM | 822 | N | LEU | 410 | 26.676 | -3.544 | 38.727 | 1.00 | 39.23 |
| | ATOM | 823 | CA | LEU | 410 | 27.931 | -3.296 | 39.423 | 1.00 | 40.45 |
| | ATOM | 824 | CB | LEU | 410 | 29.106 | -3.354 | 38.442 | 1.00 | 41.59 |
| 45 | ATOM | 825 | CG | LEU | 410 | 29.457 | -4.660 | 37.716 | 1.00 | 44.87 |
| | ATOM | 826 | CD1 | LEU | 410 | 30.972 | -4.728 | 37.554 | 1.00 | 45.41 |
| | ATOM | 827 | CD2 | LEU | 410 | 28.949 | -5.872 | 38.484 | 1.00 | 47.02 |
| | ATOM | 828 | C | LEU | 410 | 27.946 | -1.944 | 40.132 | 1.00 | 40.67 |
| | ATOM | 829 | O | LEU | 410 | 27.361 | -0.970 | 39.652 | 1.00 | 40.22 |
| 50 | ATOM | 830 | N | ASP | 411 | 28.610 | -1.890 | 41.281 | 1.00 | 41.57 |
| | ATOM | 831 | CA | ASP | 411 | 28.717 | -0.640 | 42.025 | 1.00 | 42.69 |
| | ATOM | 832 | CB | ASP | 411 | 28.490 | -0.874 | 43.528 | 1.00 | 44.44 |
| | ATOM | 833 | CG | ASP | 411 | 29.655 | -1.578 | 44.210 | 1.00 | 46.70 |
| | ATOM | 834 | OD1 | ASP | 411 | 29.537 | -1.849 | 45.426 | 1.00 | 51.44 |
| 55 | ATOM | 835 | OD2 | ASP | 411 | 30.680 | -1.861 | 43.553 | 1.00 | 48.79 |
| | ATOM | 836 | C | ASP | 411 | 30.088 | -0.016 | 41.779 | 1.00 | 43.70 |
| | ATOM | 837 | O | ASP | 411 | 30.933 | -0.610 | 41.107 | 1.00 | 38.48 |
| | ATOM | 838 | N | ARG | 412 | 30.295 | 1.181 | 42.321 | 1.00 | 46.78 |
| | ATOM | 839 | CA | ARG | 412 | 31.554 | 1.905 | 42.171 | 1.00 | 49.97 |
| 60 | ATOM | 840 | CB | ARG | 412 | 31.601 | 3.090 | 43.138 | 1.00 | 51.28 |
| | ATOM | 841 | CG | ARG | 412 | 30.971 | 4.364 | 42.614 | 1.00 | 54.77 |

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|----|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 842 | CD | ARG | 412 | 31.644 | 5.580 | 43.219 | 1.00 | 54.61 |
| | ATOM | 843 | NE | ARG | 412 | 33.071 | 5.615 | 42.912 | 1.00 | 56.53 |
| | ATOM | 844 | CZ | ARG | 412 | 33.827 | 6.708 | 42.985 | 1.00 | 61.90 |
| | ATOM | 845 | NH1 | ARG | 412 | 33.291 | 7.866 | 43.356 | 1.00 | 63.48 |
| | ATOM | 846 | NH2 | ARG | 412 | 35.120 | 6.645 | 42.682 | 1.00 | 61.21 |
| 10 | ATOM | 847 | C | ARG | 412 | 32.771 | 1.026 | 42.429 | 1.00 | 50.29 |
| | ATOM | 848 | O | ARG | 412 | 33.628 | 0.866 | 41.561 | 1.00 | 51.02 |
| | ATOM | 849 | N | ASN | 413 | 32.844 | 0.469 | 43.633 | 1.00 | 51.94 |
| | ATOM | 850 | CA | ASN | 413 | 33.969 | -0.375 | 44.021 | 1.00 | 53.15 |
| | ATOM | 851 | CB | ASN | 413 | 33.719 | -0.980 | 45.403 | 1.00 | 55.88 |
| 15 | ATOM | 852 | CG | ASN | 413 | 33.654 | 0.073 | 46.496 | 1.00 | 57.99 |
| | ATOM | 853 | OD1 | ASN | 413 | 33.697 | 1.276 | 46.223 | 1.00 | 58.27 |
| | ATOM | 854 | ND2 | ASN | 413 | 33.551 | -0.375 | 47.742 | 1.00 | 57.90 |
| | ATOM | 855 | C | ASN | 413 | 34.235 | -1.480 | 43.013 | 1.00 | 53.95 |
| | ATOM | 856 | O | ASN | 413 | 35.386 | -1.743 | 42.659 | 1.00 | 53.67 |
| 20 | ATOM | 857 | N | GLN | 414 | 33.173 | -2.129 | 42.547 | 1.00 | 55.33 |
| | ATOM | 858 | CA | GLN | 414 | 33.326 | -3.198 | 41.573 | 1.00 | 55.42 |
| | ATOM | 859 | CB | GLN | 414 | 31.991 | -3.904 | 41.343 | 1.00 | 55.44 |
| | ATOM | 860 | CG | GLN | 414 | 31.645 | -4.933 | 42.391 | 1.00 | 56.07 |
| | ATOM | 861 | CD | GLN | 414 | 30.203 | -5.376 | 42.336 | 1.00 | 57.40 |
| 25 | ATOM | 862 | OE1 | GLN | 414 | 29.296 | -4.536 | 42.402 | 1.00 | 60.22 |
| | ATOM | 863 | NE2 | GLN | 414 | 29.973 | -6.664 | 42.199 | 1.00 | 57.27 |
| | ATOM | 864 | C | GLN | 414 | 33.850 | -2.630 | 40.259 | 1.00 | 55.51 |
| | ATOM | 865 | O | GLN | 414 | 34.654 | -3.265 | 39.578 | 1.00 | 56.16 |
| | ATOM | 866 | N | GLY | 415 | 33.398 | -1.430 | 39.910 | 1.00 | 57.07 |
| 30 | ATOM | 867 | CA | GLY | 415 | 33.849 | -0.806 | 38.680 | 1.00 | 58.51 |
| | ATOM | 868 | C | GLY | 415 | 35.350 | -0.582 | 38.689 | 1.00 | 61.10 |
| | ATOM | 869 | O | GLY | 415 | 36.023 | -0.748 | 37.671 | 1.00 | 59.47 |
| | ATOM | 870 | N | LYS | 416 | 35.877 | -0.211 | 39.851 | 1.00 | 62.77 |
| | ATOM | 871 | CA | LYS | 416 | 37.305 | 0.041 | 40.011 | 1.00 | 65.49 |
| 35 | ATOM | 872 | CB | LYS | 416 | 37.634 | 0.262 | 41.491 | 1.00 | 66.04 |
| | ATOM | 873 | CG | LYS | 416 | 38.121 | 1.663 | 41.823 | 1.00 | 68.71 |
| | ATOM | 874 | CD | LYS | 416 | 37.078 | 2.439 | 42.613 | 1.00 | 70.98 |
| | ATOM | 875 | CE | LYS | 416 | 37.404 | 2.448 | 44.100 | 1.00 | 71.84 |
| | ATOM | 876 | NZ | LYS | 416 | 36.225 | 2.079 | 44.933 | 1.00 | 71.95 |
| 40 | ATOM | 877 | C | LYS | 416 | 38.159 | -1.105 | 39.472 | 1.00 | 66.41 |
| | ATOM | 878 | O | LYS | 416 | 39.361 | -0.946 | 39.269 | 1.00 | 67.15 |
| | ATOM | 879 | N | CYS | 417 | 37.538 | -2.257 | 39.238 | 1.00 | 67.33 |
| | ATOM | 880 | CA | CYS | 417 | 38.270 | -3.414 | 38.741 | 1.00 | 68.16 |
| | ATOM | 881 | CB | CYS | 417 | 37.951 | -4.642 | 39.602 | 1.00 | 70.88 |
| 45 | ATOM | 882 | SG | CYS | 417 | 38.592 | -4.549 | 41.301 | 1.00 | 76.09 |
| | ATOM | 883 | C | CYS | 417 | 38.015 | -3.736 | 37.270 | 1.00 | 67.54 |
| | ATOM | 884 | O | CYS | 417 | 38.632 | -4.653 | 36.720 | 1.00 | 68.48 |
| | ATOM | 885 | N | VAL | 418 | 37.111 | -2.994 | 36.631 | 1.00 | 64.67 |
| | ATOM | 886 | CA | VAL | 418 | 36.817 | -3.226 | 35.218 | 1.00 | 59.97 |
| 50 | ATOM | 887 | CB | VAL | 418 | 35.326 | -2.917 | 34.879 | 1.00 | 59.60 |
| | ATOM | 888 | CG1 | VAL | 418 | 34.971 | -1.503 | 35.284 | 1.00 | 59.13 |
| | ATOM | 889 | CG2 | VAL | 418 | 35.072 | -3.121 | 33.391 | 1.00 | 54.85 |
| | ATOM | 890 | C | VAL | 418 | 37.739 | -2.362 | 34.355 | 1.00 | 58.37 |
| | ATOM | 891 | O | VAL | 418 | 37.799 | -1.140 | 34.512 | 1.00 | 55.44 |
| 55 | ATOM | 892 | N | GLU | 419 | 38.463 | -3.012 | 33.450 | 1.00 | 56.02 |
| | ATOM | 893 | CA | GLU | 419 | 39.403 | -2.328 | 32.570 | 1.00 | 54.28 |
| | ATOM | 894 | CB | GLU | 419 | 40.149 | -3.351 | 31.710 | 1.00 | 57.57 |
| | ATOM | 895 | CG | GLU | 419 | 39.385 | -3.779 | 30.468 | 1.00 | 60.87 |
| | ATOM | 896 | CD | GLU | 419 | 40.179 | -4.722 | 29.584 | 1.00 | 63.34 |
| 60 | ATOM | 897 | OE1 | GLU | 419 | 40.432 | -5.870 | 30.011 | 1.00 | 64.90 |
| | ATOM | 898 | OE2 | GLU | 419 | 40.546 | -4.313 | 28.462 | 1.00 | 63.18 |

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|----|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 899 | C | GLU | 419 | 38.761 | -1.281 | 31.662 | 1.00 | 52.05 |
| | ATOM | 900 | O | GLU | 419 | 37.665 | -1.481 | 31.131 | 1.00 | 49.82 |
| | ATOM | 901 | N | GLY | 420 | 39.465 | -0.165 | 31.491 | 1.00 | 49.45 |
| | ATOM | 902 | CA | GLY | 420 | 38.983 | 0.908 | 30.642 | 1.00 | 46.22 |
| | ATOM | 903 | C | GLY | 420 | 37.895 | 1.767 | 31.254 | 1.00 | 44.55 |
| 10 | ATOM | 904 | O | GLY | 420 | 37.417 | 2.705 | 30.619 | 1.00 | 42.08 |
| | ATOM | 905 | N | MET | 421 | 37.503 | 1.471 | 32.488 | 1.00 | 43.41 |
| | ATOM | 906 | CA | MET | 421 | 36.449 | 2.248 | 33.123 | 1.00 | 42.48 |
| | ATOM | 907 | CB | MET | 421 | 35.306 | 1.327 | 33.554 | 1.00 | 42.34 |
| | ATOM | 908 | CG | MET | 421 | 34.590 | 0.635 | 32.396 | 1.00 | 38.22 |
| 15 | ATOM | 909 | SD | MET | 421 | 32.927 | 0.102 | 32.843 | 1.00 | 38.56 |
| | ATOM | 910 | CE | MET | 421 | 32.003 | 1.699 | 32.766 | 1.00 | 35.54 |
| | ATOM | 911 | C | MET | 421 | 36.923 | 3.059 | 34.312 | 1.00 | 41.64 |
| | ATOM | 912 | O | MET | 421 | 36.113 | 3.512 | 35.111 | 1.00 | 39.77 |
| | ATOM | 913 | N | VAL | 422 | 38.232 | 3.256 | 34.430 | 1.00 | 43.42 |
| 20 | ATOM | 914 | CA | VAL | 422 | 38.757 | 4.019 | 35.557 | 1.00 | 44.79 |
| | ATOM | 915 | CB | VAL | 422 | 40.285 | 4.248 | 35.433 | 1.00 | 46.54 |
| | ATOM | 916 | CG1 | VAL | 422 | 40.595 | 5.086 | 34.206 | 1.00 | 48.25 |
| | ATOM | 917 | CG2 | VAL | 422 | 40.813 | 4.920 | 36.696 | 1.00 | 46.24 |
| | ATOM | 918 | C | VAL | 422 | 38.056 | 5.372 | 35.689 | 1.00 | 44.09 |
| 25 | ATOM | 919 | O | VAL | 422 | 37.691 | 5.783 | 36.783 | 1.00 | 44.12 |
| | ATOM | 920 | N | GLU | 423 | 37.846 | 6.055 | 34.570 | 1.00 | 42.07 |
| | ATOM | 921 | CA | GLU | 423 | 37.192 | 7.356 | 34.616 | 1.00 | 40.24 |
| | ATOM | 922 | CB | GLU | 423 | 37.909 | 8.338 | 33.684 | 1.00 | 44.02 |
| | ATOM | 923 | CG | GLU | 423 | 39.411 | 8.467 | 33.893 | 1.00 | 50.04 |
| 30 | ATOM | 924 | CD | GLU | 423 | 40.096 | 9.158 | 32.719 | 1.00 | 55.64 |
| | ATOM | 925 | OE1 | GLU | 423 | 39.539 | 10.156 | 32.205 | 1.00 | 56.66 |
| | ATOM | 926 | OE2 | GLU | 423 | 41.188 | 8.703 | 32.306 | 1.00 | 58.02 |
| | ATOM | 927 | C | GLU | 423 | 35.704 | 7.337 | 34.250 | 1.00 | 35.77 |
| | ATOM | 928 | O | GLU | 423 | 34.881 | 7.955 | 34.919 | 1.00 | 33.20 |
| 35 | ATOM | 929 | N | ILE | 424 | 35.345 | 6.617 | 33.197 | 1.00 | 36.16 |
| | ATOM | 930 | CA | ILE | 424 | 33.949 | 6.643 | 32.771 | 1.00 | 31.63 |
| | ATOM | 931 | CB | ILE | 424 | 33.803 | 6.087 | 31.347 | 1.00 | 33.58 |
| | ATOM | 932 | CG2 | ILE | 424 | 34.639 | 6.936 | 30.395 | 1.00 | 33.48 |
| | ATOM | 933 | CG1 | ILE | 424 | 34.204 | 4.617 | 31.296 | 1.00 | 34.46 |
| 40 | ATOM | 934 | CD1 | ILE | 424 | 33.857 | 3.955 | 29.978 | 1.00 | 34.67 |
| | ATOM | 935 | C | ILE | 424 | 32.890 | 6.035 | 33.685 | 1.00 | 28.89 |
| | ATOM | 936 | O | ILE | 424 | 31.729 | 6.443 | 33.632 | 1.00 | 26.49 |
| | ATOM | 937 | N | PHE | 425 | 33.261 | 5.091 | 34.542 | 1.00 | 29.26 |
| | ATOM | 938 | CA | PHE | 425 | 32.257 | 4.520 | 35.447 | 1.00 | 29.87 |
| 45 | ATOM | 939 | CB | PHE | 425 | 32.903 | 3.529 | 36.423 | 1.00 | 31.26 |
| | ATOM | 940 | CG | PHE | 425 | 31.948 | 2.496 | 36.959 | 1.00 | 32.17 |
| | ATOM | 941 | CD1 | PHE | 425 | 31.124 | 2.783 | 38.048 | 1.00 | 33.70 |
| | ATOM | 942 | CD2 | PHE | 425 | 31.881 | 1.230 | 36.381 | 1.00 | 30.64 |
| | ATOM | 943 | CE1 | PHE | 425 | 30.244 | 1.814 | 38.563 | 1.00 | 32.60 |
| 50 | ATOM | 944 | CE2 | PHE | 425 | 31.010 | 0.256 | 36.881 | 1.00 | 31.55 |
| | ATOM | 945 | CZ | PHE | 425 | 30.189 | 0.549 | 37.973 | 1.00 | 33.34 |
| | ATOM | 946 | C | PHE | 425 | 31.594 | 5.649 | 36.240 | 1.00 | 30.17 |
| | ATOM | 947 | O | PHE | 425 | 30.368 | 5.774 | 36.276 | 1.00 | 26.71 |
| | ATOM | 948 | N | ASP | 426 | 32.415 | 6.483 | 36.870 | 1.00 | 29.45 |
| 55 | ATOM | 949 | CA | ASP | 426 | 31.893 | 7.587 | 37.661 | 1.00 | 32.29 |
| | ATOM | 950 | CB | ASP | 426 | 33.031 | 8.291 | 38.401 | 1.00 | 33.49 |
| | ATOM | 951 | CG | ASP | 426 | 33.455 | 7.546 | 39.655 | 1.00 | 39.42 |
| | ATOM | 952 | OD1 | ASP | 426 | 32.767 | 6.574 | 40.038 | 1.00 | 38.35 |
| | ATOM | 953 | OD2 | ASP | 426 | 34.480 | 7.934 | 40.256 | 1.00 | 39.58 |
| 60 | ATOM | 954 | C | ASP | 426 | 31.133 | 8.592 | 36.806 | 1.00 | 29.02 |
| | ATOM | 955 | O | ASP | 426 | 30.154 | 9.175 | 37.257 | 1.00 | 31.34 |

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|----|------|------|-----|------|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 956 | N | MET | 427 | 31.585 | 8.797 | 35.572 | 1.00 | 30.69 |
| | ATOM | 957 | CA | MET | 427 | 30.919 | 9.736 | 34.675 | 1.00 | 28.63 |
| | ATOM | 958 | CB | MET | 427 | 31.744 | 9.912 | 33.407 | 1.00 | 26.83 |
| | ATOM | 959 | CG | MET | 427 | 33.032 | 10.680 | 33.608 | 1.00 | 31.41 |
| | ATOM | 960 | SD | MET | 427 | 33.962 | 10.783 | 32.077 | 1.00 | 34.87 |
| 10 | ATOM | 961 | CE | MET | 427 | 35.409 | 11.753 | 32.643 | 1.00 | 44.60 |
| | ATOM | 962 | C | MET | 427 | 29.526 | 9.202 | 34.324 | 1.00 | 28.70 |
| | ATOM | 963 | O | MET | 427 | 28.536 | 9.947 | 34.302 | 1.00 | 25.01 |
| | ATOM | 964 | N | LEU | 428 | 29.451 | 7.902 | 34.057 | 1.00 | 25.13 |
| | ATOM | 965 | CA | LEU | 428 | 28.173 | 7.292 | 33.730 | 1.00 | 27.60 |
| 15 | ATOM | 966 | CB | LEU | 428 | 28.379 | 5.824 | 33.332 | 1.00 | 28.00 |
| | ATOM | 967 | CG | LEU | 428 | 29.039 | 5.682 | 31.957 | 1.00 | 26.99 |
| | ATOM | 968 | CD1 | LEU | 428 | 29.678 | 4.303 | 31.782 | 1.00 | 27.80 |
| | ATOM | 969 | CD2 | LEU | 428 | 27.995 | 5.927 | 30.894 | 1.00 | 25.33 |
| | ATOM | 970 | C | LEU | 428 | 27.210 | 7.412 | 34.916 | 1.00 | 29.59 |
| 20 | ATOM | 971 | O | LEU | 428 | 26.041 | 7.743 | 34.743 | 1.00 | 27.07 |
| | ATOM | 972 | N | LEU | 429 | 27.701 | 7.147 | 36.126 | 1.00 | 30.40 |
| | ATOM | 973 | CA | LEU | 429 | 26.859 | 7.251 | 37.323 | 1.00 | 30.59 |
| | ATOM | 974 | CB | LEU | 429 | 27.675 | 6.884 | 38.571 | 1.00 | 31.76 |
| | ATOM | 975 | CG | LEU | 429 | 28.078 | 5.415 | 38.757 | 1.00 | 32.43 |
| 25 | ATOM | 976 | CD1 | LEU | 429 | 28.961 | 5.264 | 39.995 | 1.00 | 31.60 |
| | ATOM | 977 | CD2 | LEU | 429 | 26.825 | 4.573 | 38.903 | 1.00 | 34.66 |
| | ATOM | 978 | C | LEU | 429 | 26.319 | 8.681 | 37.466 | 1.00 | 30.46 |
| | ATOM | 979 | O | LEU | 429 | 25.143 | 8.901 | 37.769 | 1.00 | 28.40 |
| | ATOM | 980 | N | ALA | 430 | 27.193 | 9.656 | 37.237 | 1.00 | 31.34 |
| 30 | ATOM | 981 | CA | ALA | 430 | 26.806 | 11.059 | 37.332 | 1.00 | 29.83 |
| | ATOM | 982 | CB | ALA | 430 | 28.017 | 11.951 | 37.078 | 1.00 | 31.29 |
| | ATOM | 983 | C | ALA | 430 | 25.696 | 11.387 | 36.344 | 1.00 | 31.04 |
| | ATOM | 984 | O | ALA | 430 | 24.753 | 12.107 | 36.674 | 1.00 | 30.79 |
| | ATOM | 985 | N | THR | 431 | 25.802 | 10.854 | 35.128 | 1.00 | 30.30 |
| 35 | ATOM | 986 | CA | THR | 431 | 24.786 | 11.105 | 34.112 | 1.00 | 28.81 |
| | ATOM | 987 | CB | THR | 431 | 25.207 | 10.533 | 32.737 | 1.00 | 30.55 |
| | ATOM | 988 | OG1 | THR | 431 | 26.569 | 10.893 | 32.465 | 1.00 | 31.88 |
| | ATOM | 989 | CG2 | THR | 431 | 24.321 | 11.087 | 31.634 | 1.00 | 25.63 |
| | ATOM | 990 | C | THR | 431 | 23.462 | 10.481 | 34.530 | 1.00 | 29.49 |
| 40 | ATOM | 991 | O | THR | 431 | 22.402 | 11.099 | 34.397 | 1.00 | 26.18 |
| | ATOM | 992 | N | SER | 432 | 23.520 | 9.253 | 35.037 | 1.00 | 28.11 |
| | ATOM | 993 | CA | SER | 432 | 22.308 | 8.573 | 35.480 | 1.00 | 29.78 |
| | ATOM | 994 | CB | SER | 432 | 22.639 | 7.177 | 36.008 | 1.00 | 33.11 |
| | ATOM | 995 | OG | SER | 432 | 21.454 | 6.412 | 36.136 | 1.00 | 36.92 |
| 45 | ATOM | 996 | C | SER | 432 | 21.651 | 9.399 | 36.589 | 1.00 | 31.49 |
| | ATOM | 997 | O | SER | 432 | 20.433 | 9.576 | 36.613 | 1.00 | 30.09 |
| | ATOM | 998 | N | ASER | 433 | 22.476 | 9.901 | 37.496 | 0.75 | 32.09 |
| | ATOM | 999 | N | BSER | 433 | 22.474 | 9.906 | 37.500 | 0.25 | 31.10 |
| | ATOM | 1000 | CA | ASER | 433 | 22.002 | 10.715 | 38.605 | 0.75 | 35.68 |
| 50 | ATOM | 1001 | CA | BSER | 433 | 21.985 | 10.717 | 38.608 | 0.25 | 32.21 |
| | ATOM | 1002 | CB | ASER | 433 | 23.185 | 11.097 | 39.502 | 0.75 | 37.18 |
| | ATOM | 1003 | CB | BSER | 433 | 23.145 | 11.104 | 39.529 | 0.25 | 31.45 |
| | ATOM | 1004 | OG | ASER | 433 | 22.823 | 12.090 | 40.443 | 0.75 | 44.09 |
| | ATOM | 1005 | OG | BSER | 433 | 23.785 | 9.953 | 40.053 | 0.25 | 29.52 |
| 55 | ATOM | 1006 | C | ASER | 433 | 21.299 | 11.971 | 38.091 | 0.75 | 35.01 |
| | ATOM | 1007 | C | BSER | 433 | 21.295 | 11.976 | 38.092 | 0.25 | 32.88 |
| | ATOM | 1008 | O | ASER | 433 | 20.257 | 12.373 | 38.612 | 0.75 | 35.34 |
| | ATOM | 1009 | O | BSER | 433 | 20.264 | 12.391 | 38.622 | 0.25 | 33.42 |
| | ATOM | 1010 | N | ARG | 434 | 21.867 | 12.579 | 37.054 | 1.00 | 33.38 |
| 60 | ATOM | 1011 | CA | ARG | 434 | 21.300 | 13.788 | 36.470 | 1.00 | 34.19 |
| | ATOM | 1012 | CB | ARG | 434 | 22.239 | 14.354 | 35.400 | 1.00 | 33.89 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1013 | CG | ARG | 434 | 21.670 | 15.528 | 34.625 | 1.00 | 38.30 |
| | ATOM | 1014 | CD | ARG | 434 | 21.559 | 16.787 | 35.479 | 1.00 | 37.91 |
| | ATOM | 1015 | NE | ARG | 434 | 21.158 | 17.944 | 34.680 | 1.00 | 37.78 |
| | ATOM | 1016 | CZ | ARG | 434 | 20.488 | 18.995 | 35.149 | 1.00 | 41.06 |
| | ATOM | 1017 | NH1 | ARG | 434 | 20.132 | 19.049 | 36.428 | 1.00 | 40.70 |
| 10 | ATOM | 1018 | NH2 | ARG | 434 | 20.175 | 19.998 | 34.337 | 1.00 | 38.78 |
| | ATOM | 1019 | C | ARG | 434 | 19.937 | 13.491 | 35.873 | 1.00 | 33.48 |
| | ATOM | 1020 | O | ARG | 434 | 18.996 | 14.266 | 36.053 | 1.00 | 30.54 |
| | ATOM | 1021 | N | PHE | 435 | 19.831 | 12.371 | 35.158 | 1.00 | 34.68 |
| | ATOM | 1022 | CA | PHE | 435 | 18.563 | 11.963 | 34.549 | 1.00 | 35.02 |
| 15 | ATOM | 1023 | CB | PHE | 435 | 18.727 | 10.634 | 33.796 | 1.00 | 34.96 |
| | ATOM | 1024 | CG | PHE | 435 | 19.240 | 10.779 | 32.386 | 1.00 | 37.63 |
| | ATOM | 1025 | CD1 | PHE | 435 | 19.459 | 12.035 | 31.824 | 1.00 | 42.03 |
| | ATOM | 1026 | CD2 | PHE | 435 | 19.521 | 9.649 | 31.623 | 1.00 | 41.24 |
| | ATOM | 1027 | CE1 | PHE | 435 | 19.953 | 12.164 | 30.521 | 1.00 | 43.11 |
| 20 | ATOM | 1028 | CE2 | PHE | 435 | 20.016 | 9.768 | 30.322 | 1.00 | 40.59 |
| | ATOM | 1029 | CZ | PHE | 435 | 20.233 | 11.029 | 29.775 | 1.00 | 40.63 |
| | ATOM | 1030 | C | PHE | 435 | 17.527 | 11.780 | 35.657 | 1.00 | 35.49 |
| | ATOM | 1031 | O | PHE | 435 | 16.361 | 12.135 | 35.496 | 1.00 | 34.78 |
| | ATOM | 1032 | N | ARG | 436 | 17.968 | 11.216 | 36.777 | 1.00 | 38.27 |
| 25 | ATOM | 1033 | CA | ARG | 436 | 17.094 | 10.982 | 37.924 | 1.00 | 40.67 |
| | ATOM | 1034 | CB | ARG | 436 | 17.844 | 10.215 | 39.012 | 1.00 | 40.70 |
| | ATOM | 1035 | CG | ARG | 436 | 16.942 | 9.590 | 40.068 | 1.00 | 44.98 |
| | ATOM | 1036 | CD | ARG | 436 | 17.648 | 8.459 | 40.810 | 1.00 | 48.09 |
| | ATOM | 1037 | NE | ARG | 436 | 18.982 | 8.841 | 41.275 | 1.00 | 50.16 |
| 30 | ATOM | 1038 | CZ | ARG | 436 | 20.119 | 8.361 | 40.777 | 1.00 | 52.19 |
| | ATOM | 1039 | NH1 | ARG | 436 | 20.099 | 7.472 | 39.790 | 1.00 | 49.34 |
| | ATOM | 1040 | NH2 | ARG | 436 | 21.283 | 8.770 | 41.266 | 1.00 | 51.85 |
| | ATOM | 1041 | C | ARG | 436 | 16.576 | 12.302 | 38.493 | 1.00 | 40.40 |
| | ATOM | 1042 | O | ARG | 436 | 15.382 | 12.458 | 38.730 | 1.00 | 41.49 |
| 35 | ATOM | 1043 | N | MET | 437 | 17.477 | 13.252 | 38.706 | 1.00 | 40.02 |
| | ATOM | 1044 | CA | MET | 437 | 17.090 | 14.546 | 39.245 | 1.00 | 41.02 |
| | ATOM | 1045 | CB | MET | 437 | 18.329 | 15.427 | 39.440 | 1.00 | 40.29 |
| | ATOM | 1046 | C | MET | 437 | 16.099 | 15.221 | 38.299 | 1.00 | 40.81 |
| | ATOM | 1047 | O | MET | 437 | 15.111 | 15.805 | 38.734 | 1.00 | 42.46 |
| 40 | ATOM | 1048 | N | MET | 438 | 16.367 | 15.127 | 37.001 | 1.00 | 39.02 |
| | ATOM | 1049 | CA | MET | 438 | 15.510 | 15.732 | 35.988 | 1.00 | 40.11 |
| | ATOM | 1050 | CB | MET | 438 | 16.237 | 15.793 | 34.651 | 1.00 | 38.16 |
| | ATOM | 1051 | CG | MET | 438 | 17.352 | 16.794 | 34.601 | 1.00 | 41.52 |
| | ATOM | 1052 | SD | MET | 438 | 17.999 | 16.862 | 32.943 | 1.00 | 43.94 |
| 45 | ATOM | 1053 | CE | MET | 438 | 16.698 | 17.748 | 32.096 | 1.00 | 39.96 |
| | ATOM | 1054 | C | MET | 438 | 14.221 | 14.964 | 35.783 | 1.00 | 37.72 |
| | ATOM | 1055 | O | MET | 438 | 13.305 | 15.451 | 35.125 | 1.00 | 36.82 |
| | ATOM | 1056 | N | ASN | 439 | 14.155 | 13.759 | 36.337 | 1.00 | 38.81 |
| | ATOM | 1057 | CA | ASN | 439 | 12.981 | 12.919 | 36.174 | 1.00 | 40.77 |
| 50 | ATOM | 1058 | CB | ASN | 439 | 11.762 | 13.556 | 36.847 | 1.00 | 44.52 |
| | ATOM | 1059 | CG | ASN | 439 | 10.566 | 12.620 | 36.887 | 1.00 | 48.29 |
| | ATOM | 1060 | OD1 | ASN | 439 | 10.721 | 11.400 | 36.964 | 1.00 | 48.48 |
| | ATOM | 1061 | ND2 | ASN | 439 | 9.365 | 13.189 | 36.829 | 1.00 | 50.23 |
| | ATOM | 1062 | C | ASN | 439 | 12.725 | 12.744 | 34.677 | 1.00 | 39.36 |
| 55 | ATOM | 1063 | O | ASN | 439 | 11.637 | 13.037 | 34.172 | 1.00 | 37.76 |
| | ATOM | 1064 | N | LEU | 440 | 13.749 | 12.274 | 33.972 | 1.00 | 37.65 |
| | ATOM | 1065 | CA | LEU | 440 | 13.655 | 12.052 | 32.532 | 1.00 | 35.22 |
| | ATOM | 1066 | CB | LEU | 440 | 14.999 | 11.576 | 31.987 | 1.00 | 34.70 |
| | ATOM | 1067 | CG | LEU | 440 | 15.022 | 11.467 | 30.462 | 1.00 | 35.45 |
| 60 | ATOM | 1068 | CD1 | LEU | 440 | 14.890 | 12.862 | 29.869 | 1.00 | 35.24 |
| | ATOM | 1069 | CD2 | LEU | 440 | 16.297 | 10.795 | 29.999 | 1.00 | 35.30 |

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|----|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| 5 | ATOM | 1070 | C | LEU | 440 | 12.587 | 11.024 | 32.4196 | 1.00 | 36.48 |
| | ATOM | 1071 | O | LEU | 440 | 12.518 | 9.967 | 32.826 | 1.00 | 37.36 |
| | ATOM | 1072 | N | GLN | 441 | 11.763 | 11.328 | 31.197 | 1.00 | 36.82 |
| | ATOM | 1073 | CA | GLN | 441 | 10.696 | 10.420 | 30.785 | 1.00 | 38.51 |
| | ATOM | 1074 | CB | GLN | 441 | 9.431 | 11.211 | 30.443 | 1.00 | 38.23 |
| 10 | ATOM | 1075 | CG | GLN | 441 | 8.912 | 12.063 | 31.592 | 1.00 | 42.46 |
| | ATOM | 1076 | CD | GLN | 441 | 8.362 | 11.227 | 32.729 | 1.00 | 44.91 |
| | ATOM | 1077 | OE1 | GLN | 441 | 7.268 | 10.668 | 32.629 | 1.00 | 47.31 |
| | ATOM | 1078 | NE2 | GLN | 441 | 9.119 | 11.132 | 33.818 | 1.00 | 44.06 |
| | ATOM | 1079 | C | GLN | 441 | 11.099 | 9.565 | 29.585 | 1.00 | 38.48 |
| 15 | ATOM | 1080 | O | GLN | 441 | 11.923 | 9.976 | 28.763 | 1.00 | 35.80 |
| | ATOM | 1081 | N | GLY | 442 | 10.500 | 8.378 | 29.494 | 1.00 | 36.03 |
| | ATOM | 1082 | CA | GLY | 442 | 10.792 | 7.468 | 28.401 | 1.00 | 37.72 |
| | ATOM | 1083 | C | GLY | 442 | 10.599 | 8.112 | 27.043 | 1.00 | 36.88 |
| | ATOM | 1084 | O | GLY | 442 | 11.381 | 7.877 | 26.123 | 1.00 | 33.72 |
| 20 | ATOM | 1085 | N | GLU | 443 | 9.556 | 8.925 | 26.918 | 1.00 | 36.59 |
| | ATOM | 1086 | CA | GLU | 443 | 9.269 | 9.603 | 25.661 | 1.00 | 37.13 |
| | ATOM | 1087 | CB | GLU | 443 | 7.956 | 10.379 | 25.764 | 1.00 | 41.57 |
| | ATOM | 1088 | CG | GLU | 443 | 6.723 | 9.488 | 25.879 | 1.00 | 47.76 |
| | ATOM | 1089 | CD | GLU | 443 | 6.483 | 9.008 | 27.302 | 1.00 | 53.96 |
| 25 | ATOM | 1090 | OE1 | GLU | 443 | 5.619 | 8.123 | 27.498 | 1.00 | 57.66 |
| | ATOM | 1091 | OE2 | GLU | 443 | 7.159 | 9.515 | 28.225 | 1.00 | 56.13 |
| | ATOM | 1092 | C | GLU | 443 | 10.408 | 10.551 | 25.311 | 1.00 | 35.27 |
| | ATOM | 1093 | O | GLU | 443 | 10.759 | 10.704 | 24.145 | 1.00 | 33.85 |
| | ATOM | 1094 | N | GLU | 444 | 10.984 | 11.179 | 26.331 | 1.00 | 32.09 |
| 30 | ATOM | 1095 | CA | GLU | 444 | 12.097 | 12.095 | 26.126 | 1.00 | 33.92 |
| | ATOM | 1096 | CB | GLU | 444 | 12.332 | 12.924 | 27.388 | 1.00 | 34.97 |
| | ATOM | 1097 | CG | GLU | 444 | 11.169 | 13.845 | 27.732 | 1.00 | 38.28 |
| | ATOM | 1098 | CD | GLU | 444 | 11.383 | 14.610 | 29.023 | 1.00 | 38.11 |
| | ATOM | 1099 | OE1 | GLU | 444 | 11.800 | 13.993 | 30.026 | 1.00 | 39.53 |
| 35 | ATOM | 1100 | OE2 | GLU | 444 | 11.132 | 15.834 | 29.036 | 1.00 | 40.77 |
| | ATOM | 1101 | C | GLU | 444 | 13.356 | 11.305 | 25.770 | 1.00 | 33.59 |
| | ATOM | 1102 | O | GLU | 444 | 14.085 | 11.670 | 24.842 | 1.00 | 33.35 |
| | ATOM | 1103 | N | PHE | 445 | 13.590 | 10.215 | 26.501 | 1.00 | 30.68 |
| | ATOM | 1104 | CA | PHE | 445 | 14.753 | 9.357 | 26.276 | 1.00 | 32.49 |
| 40 | ATOM | 1105 | CB | PHE | 445 | 14.703 | 8.139 | 27.203 | 1.00 | 29.35 |
| | ATOM | 1106 | CG | PHE | 445 | 15.667 | 7.047 | 26.828 | 1.00 | 30.78 |
| | ATOM | 1107 | CD1 | PHE | 445 | 17.036 | 7.201 | 27.030 | 1.00 | 28.25 |
| | ATOM | 1108 | CD2 | PHE | 445 | 15.205 | 5.863 | 26.266 | 1.00 | 30.62 |
| | ATOM | 1109 | CE1 | PHE | 445 | 17.933 | 6.195 | 26.675 | 1.00 | 28.67 |
| 45 | ATOM | 1110 | CE2 | PHE | 445 | 16.095 | 4.848 | 25.908 | 1.00 | 31.37 |
| | ATOM | 1111 | CZ | PHE | 445 | 17.460 | 5.015 | 26.113 | 1.00 | 30.37 |
| | ATOM | 1112 | C | PHE | 445 | 14.850 | 8.885 | 24.829 | 1.00 | 31.11 |
| | ATOM | 1113 | O | PHE | 445 | 15.924 | 8.947 | 24.221 | 1.00 | 32.20 |
| | ATOM | 1114 | N | VAL | 446 | 13.739 | 8.415 | 24.266 | 1.00 | 28.63 |
| 50 | ATOM | 1115 | CA | VAL | 446 | 13.787 | 7.943 | 22.889 | 1.00 | 27.94 |
| | ATOM | 1116 | CB | VAL | 446 | 12.478 | 7.193 | 22.478 | 1.00 | 28.48 |
| | ATOM | 1117 | CG1 | VAL | 446 | 12.318 | 5.939 | 23.343 | 1.00 | 29.61 |
| | ATOM | 1118 | CG2 | VAL | 446 | 11.265 | 8.092 | 22.607 | 1.00 | 27.23 |
| | ATOM | 1119 | C | VAL | 446 | 14.099 | 9.064 | 21.900 | 1.00 | 27.28 |
| 55 | ATOM | 1120 | O | VAL | 446 | 14.781 | 8.837 | 20.904 | 1.00 | 28.07 |
| | ATOM | 1121 | N | CYS | 447 | 13.619 | 10.275 | 22.166 | 1.00 | 28.97 |
| | ATOM | 1122 | CA | CYS | 447 | 13.919 | 11.394 | 21.272 | 1.00 | 29.14 |
| | ATOM | 1123 | CB | CYS | 447 | 13.156 | 12.653 | 21.693 | 1.00 | 28.90 |
| | ATOM | 1124 | SG | CYS | 447 | 11.389 | 12.591 | 21.309 | 1.00 | 35.68 |
| 60 | ATOM | 1125 | C | CYS | 447 | 15.420 | 11.677 | 21.328 | 1.00 | 28.03 |
| | ATOM | 1126 | O | CYS | 447 | 16.063 | 11.885 | 20.302 | 1.00 | 29.34 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1127 | N | LEU | 448 | 15.969 | 11.686 | 22.538 | 1.00 | 27.28 |
| | ATOM | 1128 | CA | LEU | 448 | 17.392 | 11.938 | 22.729 | 1.00 | 25.30 |
| | ATOM | 1129 | CB | LEU | 448 | 17.733 | 11.932 | 24.220 | 1.00 | 27.72 |
| | ATOM | 1130 | CG | LEU | 448 | 17.248 | 13.135 | 25.040 | 1.00 | 29.54 |
| | ATOM | 1131 | CD1 | LEU | 448 | 17.807 | 13.042 | 26.454 | 1.00 | 30.85 |
| 10 | ATOM | 1132 | CD2 | LEU | 448 | 17.688 | 14.434 | 24.376 | 1.00 | 30.24 |
| | ATOM | 1133 | C | LEU | 448 | 18.245 | 10.902 | 22.008 | 1.00 | 27.62 |
| | ATOM | 1134 | O | LEU | 448 | 19.207 | 11.252 | 21.327 | 1.00 | 25.10 |
| | ATOM | 1135 | N | LYS | 449 | 17.905 | 9.621 | 22.162 | 1.00 | 25.16 |
| | ATOM | 1136 | CA | LYS | 449 | 18.673 | 8.570 | 21.506 | 1.00 | 27.55 |
| 15 | ATOM | 1137 | CB | LYS | 449 | 18.135 | 7.185 | 21.900 | 1.00 | 28.99 |
| | ATOM | 1138 | CG | LYS | 449 | 19.134 | 6.052 | 21.694 | 1.00 | 34.70 |
| | ATOM | 1139 | CD | LYS | 449 | 18.737 | 4.789 | 22.459 | 1.00 | 32.67 |
| | ATOM | 1140 | CE | LYS | 449 | 17.267 | 4.419 | 22.220 | 1.00 | 31.87 |
| | ATOM | 1141 | NZ | LYS | 449 | 17.022 | 2.967 | 22.472 | 1.00 | 29.14 |
| 20 | ATOM | 1142 | C | LYS | 449 | 18.626 | 8.749 | 19.990 | 1.00 | 25.88 |
| | ATOM | 1143 | O | LYS | 449 | 19.610 | 8.489 | 19.296 | 1.00 | 25.93 |
| | ATOM | 1144 | N | SER | 450 | 17.482 | 9.197 | 19.480 | 1.00 | 26.07 |
| | ATOM | 1145 | CA | SER | 450 | 17.323 | 9.421 | 18.052 | 1.00 | 27.24 |
| | ATOM | 1146 | CB | SER | 450 | 15.857 | 9.705 | 17.721 | 1.00 | 32.24 |
| 25 | ATOM | 1147 | OG | SER | 450 | 15.098 | 8.519 | 17.779 | 1.00 | 34.94 |
| | ATOM | 1148 | C | SER | 450 | 18.176 | 10.607 | 17.618 | 1.00 | 26.78 |
| | ATOM | 1149 | O | SER | 450 | 18.763 | 10.598 | 16.535 | 1.00 | 25.85 |
| | ATOM | 1150 | N | ILE | 451 | 18.231 | 11.632 | 18.463 | 1.00 | 26.94 |
| | ATOM | 1151 | CA | ILE | 451 | 19.032 | 12.810 | 18.155 | 1.00 | 26.13 |
| 30 | ATOM | 1152 | CB | ILE | 451 | 18.950 | 13.850 | 19.291 | 1.00 | 27.72 |
| | ATOM | 1153 | CG2 | ILE | 451 | 20.019 | 14.929 | 19.101 | 1.00 | 20.53 |
| | ATOM | 1154 | CG1 | ILE | 451 | 17.553 | 14.475 | 19.322 | 1.00 | 29.49 |
| | ATOM | 1155 | CD1 | ILE | 451 | 17.377 | 15.473 | 20.447 | 1.00 | 36.24 |
| | ATOM | 1156 | C | ILE | 451 | 20.489 | 12.381 | 17.989 | 1.00 | 24.88 |
| 35 | ATOM | 1157 | O | ILE | 451 | 21.161 | 12.771 | 17.034 | 1.00 | 26.96 |
| | ATOM | 1158 | N | ILE | 452 | 20.977 | 11.582 | 18.931 | 1.00 | 22.72 |
| | ATOM | 1159 | CA | ILE | 452 | 22.359 | 11.120 | 18.880 | 1.00 | 21.95 |
| | ATOM | 1160 | CB | ILE | 452 | 22.660 | 10.155 | 20.050 | 1.00 | 23.57 |
| | ATOM | 1161 | CG2 | ILE | 452 | 23.982 | 9.435 | 19.804 | 1.00 | 22.10 |
| 40 | ATOM | 1162 | CG1 | ILE | 452 | 22.718 | 10.949 | 21.371 | 1.00 | 21.70 |
| | ATOM | 1163 | CD1 | ILE | 452 | 22.768 | 10.060 | 22.624 | 1.00 | 25.30 |
| | ATOM | 1164 | C | ILE | 452 | 22.656 | 10.419 | 17.557 | 1.00 | 23.02 |
| | ATOM | 1165 | O | ILE | 452 | 23.650 | 10.708 | 16.885 | 1.00 | 21.25 |
| | ATOM | 1166 | N | LEU | 453 | 21.779 | 9.497 | 17.173 | 1.00 | 22.83 |
| 45 | ATOM | 1167 | CA | LEU | 453 | 21.984 | 8.768 | 15.935 | 1.00 | 22.05 |
| | ATOM | 1168 | CB | LEU | 453 | 20.843 | 7.764 | 15.733 | 1.00 | 22.06 |
| | ATOM | 1169 | CG | LEU | 453 | 20.712 | 7.189 | 14.324 | 1.00 | 22.03 |
| | ATOM | 1170 | CD1 | LEU | 453 | 21.815 | 6.165 | 14.107 | 1.00 | 24.81 |
| | ATOM | 1171 | CD2 | LEU | 453 | 19.328 | 6.535 | 14.156 | 1.00 | 24.73 |
| 50 | ATOM | 1172 | C | LEU | 453 | 22.092 | 9.687 | 14.717 | 1.00 | 23.95 |
| | ATOM | 1173 | O | LEU | 453 | 22.962 | 9.501 | 13.860 | 1.00 | 24.60 |
| | ATOM | 1174 | N | LEU | 454 | 21.220 | 10.687 | 14.638 | 1.00 | 26.72 |
| | ATOM | 1175 | CA | LEU | 454 | 21.234 | 11.599 | 13.494 | 1.00 | 26.45 |
| | ATOM | 1176 | CB | LEU | 454 | 19.852 | 12.242 | 13.330 | 1.00 | 25.51 |
| 55 | ATOM | 1177 | CG | LEU | 454 | 18.737 | 11.222 | 13.052 | 1.00 | 30.16 |
| | ATOM | 1178 | CD1 | LEU | 454 | 17.405 | 11.926 | 12.955 | 1.00 | 28.76 |
| | ATOM | 1179 | CD2 | LEU | 454 | 19.037 | 10.478 | 11.759 | 1.00 | 32.59 |
| | ATOM | 1180 | C | LEU | 454 | 22.292 | 12.703 | 13.552 | 1.00 | 28.24 |
| | ATOM | 1181 | O | LEU | 454 | 22.778 | 13.148 | 12.513 | 1.00 | 29.06 |
| 60 | ATOM | 1182 | N | ASN | 455 | 22.638 | 13.146 | 14.757 | 1.00 | 26.56 |
| | ATOM | 1183 | CA | ASN | 455 | 23.604 | 14.236 | 14.934 | 1.00 | 26.79 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1184 | CB | ASN | 455 | 23.284 | 14.998 | 16.224 | 1.00 | 26.20 |
| | ATOM | 1185 | CG | ASN | 455 | 24.174 | 16.217 | 16.419 | 1.00 | 27.26 |
| | ATOM | 1186 | OD1 | ASN | 455 | 24.171 | 17.134 | 15.602 | 1.00 | 30.83 |
| | ATOM | 1187 | ND2 | ASN | 455 | 24.931 | 16.230 | 17.506 | 1.00 | 27.16 |
| | ATOM | 1188 | C | ASN | 455 | 25.062 | 13.782 | 14.954 | 1.00 | 30.63 |
| 10 | ATOM | 1189 | O | ASN | 455 | 25.965 | 14.517 | 14.525 | 1.00 | 27.69 |
| | ATOM | 1190 | N | SER | 456 | 25.268 | 12.569 | 15.461 | 1.00 | 30.48 |
| | ATOM | 1191 | CA | SER | 456 | 26.572 | 11.928 | 15.579 | 1.00 | 35.26 |
| | ATOM | 1192 | CB | SER | 456 | 26.393 | 10.393 | 15.505 | 1.00 | 39.69 |
| | ATOM | 1193 | OG | SER | 456 | 25.871 | 9.953 | 14.243 | 1.00 | 30.73 |
| 15 | ATOM | 1194 | C | SER | 456 | 27.627 | 12.344 | 14.562 | 1.00 | 35.56 |
| | ATOM | 1195 | O | SER | 456 | 28.599 | 13.041 | 14.884 | 1.00 | 33.00 |
| | ATOM | 1196 | N | GLY | 457 | 27.437 | 11.886 | 13.334 | 1.00 | 33.88 |
| | ATOM | 1197 | CA | GLY | 457 | 28.393 | 12.189 | 12.292 | 1.00 | 36.77 |
| | ATOM | 1198 | C | GLY | 457 | 27.876 | 13.017 | 11.136 | 1.00 | 37.02 |
| 20 | ATOM | 1199 | O | GLY | 457 | 28.310 | 12.805 | 10.013 | 1.00 | 38.66 |
| | ATOM | 1200 | N | VAL | 458 | 26.967 | 13.956 | 11.392 | 1.00 | 39.12 |
| | ATOM | 1201 | CA | VAL | 458 | 26.438 | 14.802 | 10.317 | 1.00 | 43.81 |
| | ATOM | 1202 | CB | VAL | 458 | 25.231 | 15.648 | 10.755 | 1.00 | 44.25 |
| | ATOM | 1203 | CG1 | VAL | 458 | 24.209 | 15.713 | 9.631 | 1.00 | 44.51 |
| 25 | ATOM | 1204 | CG2 | VAL | 458 | 24.638 | 15.098 | 12.013 | 1.00 | 50.53 |
| | ATOM | 1205 | C | VAL | 458 | 27.472 | 15.801 | 9.817 | 1.00 | 46.72 |
| | ATOM | 1206 | O | VAL | 458 | 27.391 | 16.265 | 8.681 | 1.00 | 47.08 |
| | ATOM | 1207 | N | TYR | 459 | 28.432 | 16.144 | 10.670 | 1.00 | 50.74 |
| | ATOM | 1208 | CA | TYR | 459 | 29.456 | 17.114 | 10.301 | 1.00 | 55.43 |
| 30 | ATOM | 1209 | CB | TYR | 459 | 29.647 | 18.129 | 11.433 | 1.00 | 56.62 |
| | ATOM | 1210 | CG | TYR | 459 | 28.375 | 18.870 | 11.781 | 1.00 | 59.34 |
| | ATOM | 1211 | CD1 | TYR | 459 | 28.094 | 19.229 | 13.095 | 1.00 | 60.73 |
| | ATOM | 1212 | CE1 | TYR | 459 | 26.900 | 19.867 | 13.429 | 1.00 | 62.14 |
| | ATOM | 1213 | CD2 | TYR | 459 | 27.430 | 19.175 | 10.795 | 1.00 | 62.16 |
| 35 | ATOM | 1214 | CE2 | TYR | 459 | 26.234 | 19.812 | 11.118 | 1.00 | 63.83 |
| | ATOM | 1215 | CZ | TYR | 459 | 25.976 | 20.154 | 12.437 | 1.00 | 62.88 |
| | ATOM | 1216 | OH | TYR | 459 | 24.790 | 20.764 | 12.767 | 1.00 | 62.56 |
| | ATOM | 1217 | C | TYR | 459 | 30.791 | 16.489 | 9.928 | 1.00 | 57.21 |
| | ATOM | 1218 | O | TYR | 459 | 31.793 | 17.189 | 9.798 | 1.00 | 56.86 |
| 40 | ATOM | 1219 | N | THR | 460 | 30.800 | 15.173 | 9.750 | 1.00 | 59.22 |
| | ATOM | 1220 | CA | THR | 460 | 32.018 | 14.474 | 9.366 | 1.00 | 62.25 |
| | ATOM | 1221 | CB | THR | 460 | 32.502 | 13.531 | 10.499 | 1.00 | 63.07 |
| | ATOM | 1222 | OG1 | THR | 460 | 33.474 | 12.613 | 9.983 | 1.00 | 67.80 |
| | ATOM | 1223 | CG2 | THR | 460 | 31.344 | 12.759 | 11.084 | 1.00 | 60.23 |
| 45 | ATOM | 1224 | C | THR | 460 | 31.759 | 13.678 | 8.086 | 1.00 | 63.54 |
| | ATOM | 1225 | O | THR | 460 | 32.457 | 12.708 | 7.782 | 1.00 | 63.91 |
| | ATOM | 1226 | N | PHE | 461 | 30.758 | 14.113 | 7.326 | 1.00 | 65.06 |
| | ATOM | 1227 | CA | PHE | 461 | 30.395 | 13.446 | 6.080 | 1.00 | 67.00 |
| | ATOM | 1228 | CB | PHE | 461 | 29.052 | 13.975 | 5.563 | 1.00 | 66.48 |
| 50 | ATOM | 1229 | CG | PHE | 461 | 27.867 | 13.147 | 5.991 | 1.00 | 66.30 |
| | ATOM | 1230 | CD1 | PHE | 461 | 26.657 | 13.754 | 6.312 | 1.00 | 65.58 |
| | ATOM | 1231 | CD2 | PHE | 461 | 27.963 | 11.760 | 6.085 | 1.00 | 66.41 |
| | ATOM | 1232 | CE1 | PHE | 461 | 25.562 | 12.996 | 6.723 | 1.00 | 65.45 |
| | ATOM | 1233 | CE2 | PHE | 461 | 26.872 | 10.994 | 6.494 | 1.00 | 66.83 |
| 55 | ATOM | 1234 | CZ | PHE | 461 | 25.670 | 11.616 | 6.814 | 1.00 | 65.12 |
| | ATOM | 1235 | C | PHE | 461 | 31.463 | 13.604 | 5.004 | 1.00 | 68.38 |
| | ATOM | 1236 | O | PHE | 461 | 32.181 | 14.606 | 4.962 | 1.00 | 68.98 |
| | ATOM | 1237 | N | LEU | 462 | 31.542 | 12.601 | 4.132 | 1.00 | 69.57 |
| | ATOM | 1238 | CA | LEU | 462 | 32.511 | 12.545 | 3.039 | 1.00 | 71.68 |
| 60 | ATOM | 1239 | CB | LEU | 462 | 32.080 | 11.475 | 2.030 | 1.00 | 71.00 |
| | ATOM | 1240 | C | LEU | 462 | 32.810 | 13.856 | 2.304 | 1.00 | 72.40 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1241 | O | LEU | 462 | 33.725 | 14.590 | 2.680 | 1.00 | 73.45 |
| | ATOM | 1242 | N | SER | 463 | 32.043 | 14.141 | 1.253 | 1.00 | 73.22 |
| | ATOM | 1243 | CA | SER | 463 | 32.262 | 15.343 | 0.449 | 1.00 | 72.61 |
| | ATOM | 1244 | CB | SER | 463 | 32.544 | 14.942 | -1.005 | 1.00 | 73.38 |
| | ATOM | 1245 | C | SER | 463 | 31.126 | 16.362 | 0.491 | 1.00 | 71.17 |
| 10 | ATOM | 1246 | O | SER | 463 | 30.455 | 16.528 | 1.511 | 1.00 | 72.05 |
| | ATOM | 1247 | N | SER | 464 | 30.932 | 17.049 | -0.633 | 1.00 | 68.86 |
| | ATOM | 1248 | CA | SER | 464 | 29.892 | 18.063 | -0.759 | 1.00 | 66.06 |
| | ATOM | 1249 | CB | SER | 464 | 30.514 | 19.457 | -0.704 | 1.00 | 66.26 |
| | ATOM | 1250 | C | SER | 464 | 29.108 | 17.887 | -2.060 | 1.00 | 63.72 |
| 15 | ATOM | 1251 | O | SER | 464 | 28.657 | 18.862 | -2.662 | 1.00 | 62.88 |
| | ATOM | 1252 | N | THR | 465 | 28.954 | 16.638 | -2.493 | 1.00 | 60.93 |
| | ATOM | 1253 | CA | THR | 465 | 28.205 | 16.343 | -3.709 | 1.00 | 57.47 |
| | ATOM | 1254 | CB | THR | 465 | 28.185 | 14.824 | -4.004 | 1.00 | 57.80 |
| | ATOM | 1255 | OG1 | THR | 465 | 27.525 | 14.135 | -2.934 | 1.00 | 54.75 |
| 20 | ATOM | 1256 | CG2 | THR | 465 | 29.606 | 14.287 | -4.149 | 1.00 | 57.49 |
| | ATOM | 1257 | C | THR | 465 | 26.767 | 16.824 | -3.523 | 1.00 | 54.93 |
| | ATOM | 1258 | O | THR | 465 | 26.349 | 17.129 | -2.407 | 1.00 | 54.26 |
| | ATOM | 1259 | N | LEU | 466 | 26.013 | 16.892 | -4.614 | 1.00 | 51.85 |
| | ATOM | 1260 | CA | LEU | 466 | 24.625 | 17.330 | -4.550 | 1.00 | 49.25 |
| 25 | ATOM | 1261 | CB | LEU | 466 | 24.013 | 17.349 | -5.956 | 1.00 | 48.74 |
| | ATOM | 1262 | CG | LEU | 466 | 22.953 | 18.415 | -6.253 | 1.00 | 48.72 |
| | ATOM | 1263 | CD1 | LEU | 466 | 22.156 | 18.002 | -7.482 | 1.00 | 48.32 |
| | ATOM | 1264 | CD2 | LEU | 466 | 22.033 | 18.594 | -5.057 | 1.00 | 48.14 |
| | ATOM | 1265 | C | LEU | 466 | 23.817 | 16.397 | -3.650 | 1.00 | 48.16 |
| 30 | ATOM | 1266 | O | LEU | 466 | 22.961 | 16.845 | -2.883 | 1.00 | 45.90 |
| | ATOM | 1267 | N | LYS | 467 | 24.093 | 15.099 | -3.750 | 1.00 | 46.47 |
| | ATOM | 1268 | CA | LYS | 467 | 23.399 | 14.100 | -2.947 | 1.00 | 47.45 |
| | ATOM | 1269 | CB | LYS | 467 | 23.802 | 12.693 | -3.395 | 1.00 | 49.38 |
| | ATOM | 1270 | CG | LYS | 467 | 22.829 | 11.602 | -2.974 | 1.00 | 52.70 |
| 35 | ATOM | 1271 | CD | LYS | 467 | 23.561 | 10.301 | -2.682 | 1.00 | 56.48 |
| | ATOM | 1272 | CE | LYS | 467 | 23.105 | 9.180 | -3.604 | 1.00 | 59.54 |
| | ATOM | 1273 | NZ | LYS | 467 | 24.150 | 8.117 | -3.732 | 1.00 | 61.22 |
| | ATOM | 1274 | C | LYS | 467 | 23.738 | 14.284 | -1.472 | 1.00 | 46.89 |
| | ATOM | 1275 | O | LYS | 467 | 22.884 | 14.108 | -0.604 | 1.00 | 46.06 |
| 40 | ATOM | 1276 | N | SER | 468 | 24.989 | 14.644 | -1.202 | 1.00 | 45.82 |
| | ATOM | 1277 | CA | SER | 468 | 25.457 | 14.854 | 0.160 | 1.00 | 46.82 |
| | ATOM | 1278 | CB | SER | 468 | 26.976 | 15.050 | 0.173 | 1.00 | 47.85 |
| | ATOM | 1279 | OG | SER | 468 | 27.407 | 15.537 | 1.435 | 1.00 | 55.73 |
| | ATOM | 1280 | C | SER | 468 | 24.778 | 16.063 | 0.790 | 1.00 | 44.24 |
| 45 | ATOM | 1281 | O | SER | 468 | 24.473 | 16.062 | 1.983 | 1.00 | 42.98 |
| | ATOM | 1282 | N | LEU | 469 | 24.547 | 17.100 | -0.011 | 1.00 | 42.33 |
| | ATOM | 1283 | CA | LEU | 469 | 23.890 | 18.301 | 0.486 | 1.00 | 40.42 |
| | ATOM | 1284 | CB | LEU | 469 | 24.002 | 19.427 | -0.545 | 1.00 | 44.47 |
| | ATOM | 1285 | CG | LEU | 469 | 25.438 | 19.874 | -0.849 | 1.00 | 46.70 |
| 50 | ATOM | 1286 | CD1 | LEU | 469 | 25.514 | 20.477 | -2.246 | 1.00 | 46.70 |
| | ATOM | 1287 | CD2 | LEU | 469 | 25.890 | 20.883 | 0.199 | 1.00 | 47.32 |
| | ATOM | 1288 | C | LEU | 469 | 22.423 | 17.996 | 0.786 | 1.00 | 39.06 |
| | ATOM | 1289 | O | LEU | 469 | 21.856 | 18.505 | 1.760 | 1.00 | 34.97 |
| | ATOM | 1290 | N | GLU | 470 | 21.814 | 17.151 | -0.046 | 1.00 | 35.46 |
| 55 | ATOM | 1291 | CA | GLU | 470 | 20.418 | 16.768 | 0.145 | 1.00 | 34.38 |
| | ATOM | 1292 | CB | GLU | 470 | 19.914 | 15.963 | -1.052 | 1.00 | 38.02 |
| | ATOM | 1293 | CG | GLU | 470 | 19.772 | 16.773 | -2.329 | 1.00 | 42.67 |
| | ATOM | 1294 | CD | GLU | 470 | 19.339 | 15.923 | -3.509 | 1.00 | 48.30 |
| | ATOM | 1295 | OE1 | GLU | 470 | 19.671 | 14.716 | -3.538 | 1.00 | 50.53 |
| 60 | ATOM | 1296 | OE2 | GLU | 470 | 18.666 | 16.463 | -4.412 | 1.00 | 51.06 |
| | ATOM | 1297 | C | GLU | 470 | 20.290 | 15.916 | 1.403 | 1.00 | 34.37 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1298 | O | GLU | 470 | 19.321 | 16.035 | 2.157 | 1.00 | 32.60 |
| | ATOM | 1299 | N | GLU | 471 | 21.274 | 15.046 | 1.606 | 1.00 | 34.66 |
| | ATOM | 1300 | CA | GLU | 471 | 21.309 | 14.162 | 2.766 | 1.00 | 35.68 |
| | ATOM | 1301 | CB | GLU | 471 | 22.515 | 13.222 | 2.671 | 1.00 | 34.57 |
| | ATOM | 1302 | CG | GLU | 471 | 22.376 | 12.122 | 1.614 | 1.00 | 37.98 |
| 10 | ATOM | 1303 | CD | GLU | 471 | 21.476 | 10.989 | 2.063 | 1.00 | 39.79 |
| | ATOM | 1304 | OE1 | GLU | 471 | 20.268 | 11.027 | 1.743 | 1.00 | 41.12 |
| | ATOM | 1305 | OE2 | GLU | 471 | 21.974 | 10.061 | 2.737 | 1.00 | 32.11 |
| | ATOM | 1306 | C | GLU | 471 | 21.393 | 14.983 | 4.052 | 1.00 | 34.79 |
| | ATOM | 1307 | O | GLU | 471 | 20.596 | 14.793 | 4.969 | 1.00 | 32.80 |
| 15 | ATOM | 1308 | N | LYS | 472 | 22.358 | 15.898 | 4.112 | 1.00 | 33.93 |
| | ATOM | 1309 | CA | LYS | 472 | 22.518 | 16.739 | 5.291 | 1.00 | 35.58 |
| | ATOM | 1310 | CB | LYS | 472 | 23.683 | 17.710 | 5.097 | 1.00 | 39.11 |
| | ATOM | 1311 | CG | LYS | 472 | 25.050 | 17.050 | 5.138 | 1.00 | 41.47 |
| | ATOM | 1312 | CD | LYS | 472 | 26.080 | 17.957 | 5.794 | 1.00 | 46.97 |
| 20 | ATOM | 1313 | CE | LYS | 472 | 27.445 | 17.286 | 5.862 | 1.00 | 48.40 |
| | ATOM | 1314 | NZ | LYS | 472 | 27.850 | 16.702 | 4.547 | 1.00 | 51.55 |
| | ATOM | 1315 | C | LYS | 472 | 21.237 | 17.523 | 5.582 | 1.00 | 34.78 |
| | ATOM | 1316 | O | LYS | 472 | 20.795 | 17.607 | 6.724 | 1.00 | 33.95 |
| | ATOM | 1317 | N | ASP | 473 | 20.643 | 18.097 | 4.545 | 1.00 | 33.47 |
| 25 | ATOM | 1318 | CA | ASP | 473 | 19.420 | 18.865 | 4.720 | 1.00 | 34.63 |
| | ATOM | 1319 | CB | ASP | 473 | 18.923 | 19.404 | 3.380 | 1.00 | 37.21 |
| | ATOM | 1320 | CG | ASP | 473 | 17.654 | 20.221 | 3.522 | 1.00 | 43.24 |
| | ATOM | 1321 | OD1 | ASP | 473 | 16.559 | 19.687 | 3.230 | 1.00 | 45.20 |
| | ATOM | 1322 | OD2 | ASP | 473 | 17.750 | 21.396 | 3.932 | 1.00 | 45.59 |
| 30 | ATOM | 1323 | C | ASP | 473 | 18.339 | 17.998 | 5.338 | 1.00 | 32.93 |
| | ATOM | 1324 | O | ASP | 473 | 17.642 | 18.416 | 6.264 | 1.00 | 32.87 |
| | ATOM | 1325 | N | HIS | 474 | 18.199 | 16.784 | 4.827 | 1.00 | 32.74 |
| | ATOM | 1326 | CA | HIS | 474 | 17.185 | 15.882 | 5.343 | 1.00 | 32.21 |
| | ATOM | 1327 | CB | HIS | 474 | 17.185 | 14.575 | 4.568 | 1.00 | 32.79 |
| 35 | ATOM | 1328 | CG | HIS | 474 | 16.047 | 13.675 | 4.924 | 1.00 | 36.22 |
| | ATOM | 1329 | CD2 | HIS | 474 | 14.711 | 13.813 | 4.750 | 1.00 | 38.33 |
| | ATOM | 1330 | ND1 | HIS | 474 | 16.227 | 12.456 | 5.542 | 1.00 | 38.97 |
| | ATOM | 1331 | CE1 | HIS | 474 | 15.053 | 11.883 | 5.732 | 1.00 | 37.99 |
| | ATOM | 1332 | NE2 | HIS | 474 | 14.116 | 12.686 | 5.261 | 1.00 | 37.43 |
| 40 | ATOM | 1333 | C | HIS | 474 | 17.403 | 15.573 | 6.815 | 1.00 | 29.74 |
| | ATOM | 1334 | O | HIS | 474 | 16.460 | 15.543 | 7.596 | 1.00 | 29.90 |
| | ATOM | 1335 | N | ILE | 475 | 18.653 | 15.326 | 7.185 | 1.00 | 27.80 |
| | ATOM | 1336 | CA | ILE | 475 | 18.971 | 15.014 | 8.571 | 1.00 | 25.61 |
| | ATOM | 1337 | CB | ILE | 475 | 20.478 | 14.708 | 8.720 | 1.00 | 25.59 |
| 45 | ATOM | 1338 | CG2 | ILE | 475 | 20.877 | 14.713 | 10.193 | 1.00 | 27.17 |
| | ATOM | 1339 | CG1 | ILE | 475 | 20.787 | 13.341 | 8.092 | 1.00 | 26.17 |
| | ATOM | 1340 | CD1 | ILE | 475 | 22.258 | 13.071 | 7.849 | 1.00 | 27.07 |
| | ATOM | 1341 | C | ILE | 475 | 18.576 | 16.201 | 9.460 | 1.00 | 27.91 |
| | ATOM | 1342 | O | ILE | 475 | 17.928 | 16.038 | 10.485 | 1.00 | 29.16 |
| 50 | ATOM | 1343 | N | HIS | 476 | 18.956 | 17.404 | 9.054 | 1.00 | 29.41 |
| | ATOM | 1344 | CA | HIS | 476 | 18.621 | 18.575 | 9.846 | 1.00 | 29.73 |
| | ATOM | 1345 | CB | HIS | 476 | 19.342 | 19.796 | 9.281 | 1.00 | 32.27 |
| | ATOM | 1346 | CG | HIS | 476 | 20.777 | 19.867 | 9.699 | 1.00 | 39.44 |
| | ATOM | 1347 | CD2 | HIS | 476 | 21.355 | 19.707 | 10.915 | 1.00 | 39.81 |
| 55 | ATOM | 1348 | ND1 | HIS | 476 | 21.809 | 20.067 | 8.808 | 1.00 | 39.79 |
| | ATOM | 1349 | CE1 | HIS | 476 | 22.959 | 20.027 | 9.456 | 1.00 | 39.98 |
| | ATOM | 1350 | NE2 | HIS | 476 | 22.712 | 19.809 | 10.735 | 1.00 | 40.26 |
| | ATOM | 1351 | C | HIS | 476 | 17.120 | 18.810 | 9.948 | 1.00 | 31.40 |
| | ATOM | 1352 | O | HIS | 476 | 16.636 | 19.336 | 10.951 | 1.00 | 29.79 |
| 60 | ATOM | 1353 | N | ARG | 477 | 16.374 | 18.396 | 8.929 | 1.00 | 31.82 |
| | ATOM | 1354 | CA | ARG | 477 | 14.929 | 18.570 | 8.956 | 1.00 | 31.53 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1355 | CB | ARG | 477 | 14.343 | 18.376 | 7.557 | 1.00 | 34.95 |
| | ATOM | 1356 | CG | ARG | 477 | 14.425 | 19.627 | 6.700 | 1.00 | 40.46 |
| | ATOM | 1357 | CD | ARG | 477 | 13.698 | 19.445 | 5.370 | 1.00 | 45.22 |
| | ATOM | 1358 | NE | ARG | 477 | 14.107 | 20.456 | 4.399 | 1.00 | 53.05 |
| | ATOM | 1359 | CZ | ARG | 477 | 13.647 | 21.705 | 4.376 | 1.00 | 55.89 |
| 10 | ATOM | 1360 | NH1 | ARG | 477 | 12.756 | 22.106 | 5.274 | 1.00 | 56.17 |
| | ATOM | 1361 | NH2 | ARG | 477 | 14.084 | 22.558 | 3.457 | 1.00 | 59.49 |
| | ATOM | 1362 | C | ARG | 477 | 14.310 | 17.582 | 9.931 | 1.00 | 30.70 |
| | ATOM | 1363 | O | ARG | 477 | 13.360 | 17.903 | 10.649 | 1.00 | 30.24 |
| | ATOM | 1364 | N | VAL | 478 | 14.863 | 16.375 | 9.972 | 1.00 | 29.67 |
| 15 | ATOM | 1365 | CA | VAL | 478 | 14.351 | 15.369 | 10.887 | 1.00 | 29.68 |
| | ATOM | 1366 | CB | VAL | 478 | 14.937 | 13.975 | 10.575 | 1.00 | 32.01 |
| | ATOM | 1367 | CG1 | VAL | 478 | 14.461 | 12.973 | 11.609 | 1.00 | 32.93 |
| | ATOM | 1368 | CG2 | VAL | 478 | 14.506 | 13.528 | 9.169 | 1.00 | 31.00 |
| | ATOM | 1369 | C | VAL | 478 | 14.696 | 15.774 | 12.316 | 1.00 | 29.81 |
| 20 | ATOM | 1370 | O | VAL | 478 | 13.860 | 15.677 | 13.220 | 1.00 | 30.25 |
| | ATOM | 1371 | N | LEU | 479 | 15.929 | 16.232 | 12.516 | 1.00 | 28.81 |
| | ATOM | 1372 | CA | LEU | 479 | 16.360 | 16.674 | 13.836 | 1.00 | 28.74 |
| | ATOM | 1373 | CB | LEU | 479 | 17.799 | 17.210 | 13.779 | 1.00 | 26.65 |
| | ATOM | 1374 | CG | LEU | 479 | 18.910 | 16.152 | 13.853 | 1.00 | 26.05 |
| 25 | ATOM | 1375 | CD1 | LEU | 479 | 20.231 | 16.772 | 13.395 | 1.00 | 25.81 |
| | ATOM | 1376 | CD2 | LEU | 479 | 19.028 | 15.603 | 15.277 | 1.00 | 25.34 |
| | ATOM | 1377 | C | LEU | 479 | 15.411 | 17.777 | 14.313 | 1.00 | 29.54 |
| | ATOM | 1378 | O | LEU | 479 | 14.997 | 17.786 | 15.472 | 1.00 | 29.00 |
| | ATOM | 1379 | N | ASP | 480 | 15.076 | 18.703 | 13.415 | 1.00 | 31.52 |
| 30 | ATOM | 1380 | CA | ASP | 480 | 14.162 | 19.800 | 13.741 | 1.00 | 33.84 |
| | ATOM | 1381 | CB | ASP | 480 | 13.943 | 20.712 | 12.528 | 1.00 | 34.37 |
| | ATOM | 1382 | CG | ASP | 480 | 15.055 | 21.743 | 12.345 | 1.00 | 36.26 |
| | ATOM | 1383 | OD1 | ASP | 480 | 15.119 | 22.354 | 11.257 | 1.00 | 36.56 |
| | ATOM | 1384 | OD2 | ASP | 480 | 15.860 | 21.951 | 13.274 | 1.00 | 34.19 |
| 35 | ATOM | 1385 | C | ASP | 480 | 12.818 | 19.222 | 14.174 | 1.00 | 33.48 |
| | ATOM | 1386 | O | ASP | 480 | 12.186 | 19.724 | 15.105 | 1.00 | 33.89 |
| | ATOM | 1387 | N | LYS | 481 | 12.379 | 18.161 | 13.498 | 1.00 | 33.90 |
| | ATOM | 1388 | CA | LYS | 481 | 11.106 | 17.536 | 13.839 | 1.00 | 32.97 |
| | ATOM | 1389 | CB | LYS | 481 | 10.719 | 16.489 | 12.784 | 1.00 | 34.66 |
| 40 | ATOM | 1390 | C | LYS | 481 | 11.164 | 16.895 | 15.225 | 1.00 | 33.57 |
| | ATOM | 1391 | O | LYS | 481 | 10.167 | 16.869 | 15.943 | 1.00 | 35.37 |
| | ATOM | 1392 | N | ILE | 482 | 12.328 | 16.377 | 15.607 | 1.00 | 32.71 |
| | ATOM | 1393 | CA | ILE | 482 | 12.457 | 15.764 | 16.922 | 1.00 | 31.60 |
| | ATOM | 1394 | CB | ILE | 482 | 13.743 | 14.913 | 17.028 | 1.00 | 32.65 |
| 45 | ATOM | 1395 | CG2 | ILE | 482 | 13.877 | 14.338 | 18.430 | 1.00 | 32.50 |
| | ATOM | 1396 | CG1 | ILE | 482 | 13.697 | 13.785 | 15.995 | 1.00 | 32.72 |
| | ATOM | 1397 | CD1 | ILE | 482 | 14.978 | 12.969 | 15.908 | 1.00 | 33.37 |
| | ATOM | 1398 | C | ILE | 482 | 12.456 | 16.853 | 17.994 | 1.00 | 31.69 |
| | ATOM | 1399 | O | ILE | 482 | 11.946 | 16.649 | 19.097 | 1.00 | 29.98 |
| 50 | ATOM | 1400 | N | THR | 483 | 13.027 | 18.012 | 17.679 | 1.00 | 31.33 |
| | ATOM | 1401 | CA | THR | 483 | 13.022 | 19.109 | 18.644 | 1.00 | 31.71 |
| | ATOM | 1402 | CB | THR | 483 | 13.756 | 20.351 | 18.109 | 1.00 | 32.92 |
| | ATOM | 1403 | OG1 | THR | 483 | 15.111 | 20.012 | 17.788 | 1.00 | 29.99 |
| | ATOM | 1404 | CG2 | THR | 483 | 13.756 | 21.452 | 19.160 | 1.00 | 30.47 |
| 55 | ATOM | 1405 | C | THR | 483 | 11.559 | 19.483 | 18.920 | 1.00 | 32.85 |
| | ATOM | 1406 | O | THR | 483 | 11.146 | 19.598 | 20.070 | 1.00 | 31.83 |
| | ATOM | 1407 | N | ASP | 484 | 10.785 | 19.656 | 17.851 | 1.00 | 31.91 |
| | ATOM | 1408 | CA | ASP | 484 | 9.369 | 20.003 | 17.965 | 1.00 | 34.15 |
| | ATOM | 1409 | CB | ASP | 484 | 8.708 | 20.013 | 16.591 | 1.00 | 37.41 |
| 60 | ATOM | 1410 | CG | ASP | 484 | 9.270 | 21.080 | 15.680 | 1.00 | 42.02 |
| | ATOM | 1411 | OD1 | ASP | 484 | 9.871 | 22.045 | 16.198 | 1.00 | 43.26 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1412 | OD2 | ASP | 484 | 9.106 | 20.952 | 14.445 | 1.00 | 42.49 |
| | ATOM | 1413 | C | ASP | 484 | 8.657 | 18.985 | 18.840 | 1.00 | 33.16 |
| | ATOM | 1414 | O | ASP | 484 | 7.830 | 19.339 | 19.676 | 1.00 | 34.86 |
| | ATOM | 1415 | N | THR | 485 | 8.996 | 17.715 | 18.646 | 1.00 | 33.91 |
| | ATOM | 1416 | CA | THR | 485 | 8.396 | 16.635 | 19.414 | 1.00 | 34.41 |
| 10 | ATOM | 1417 | CB | THR | 485 | 8.875 | 15.268 | 18.885 | 1.00 | 33.58 |
| | ATOM | 1418 | OG1 | THR | 485 | 8.400 | 15.094 | 17.542 | 1.00 | 37.04 |
| | ATOM | 1419 | CG2 | THR | 485 | 8.347 | 14.138 | 19.751 | 1.00 | 30.89 |
| | ATOM | 1420 | C | THR | 485 | 8.708 | 16.757 | 20.903 | 1.00 | 35.15 |
| | ATOM | 1421 | O | THR | 485 | 7.818 | 16.600 | 21.744 | 1.00 | 31.99 |
| 15 | ATOM | 1422 | N | LEU | 486 | 9.966 | 17.046 | 21.229 | 1.00 | 33.77 |
| | ATOM | 1423 | CA | LEU | 486 | 10.368 | 17.192 | 22.621 | 1.00 | 34.31 |
| | ATOM | 1424 | CB | LEU | 486 | 11.879 | 17.448 | 22.721 | 1.00 | 32.00 |
| | ATOM | 1425 | CG | LEU | 486 | 12.776 | 16.201 | 22.754 | 1.00 | 34.99 |
| | ATOM | 1426 | CD1 | LEU | 486 | 14.233 | 16.613 | 22.521 | 1.00 | 32.65 |
| 20 | ATOM | 1427 | CD2 | LEU | 486 | 12.635 | 15.481 | 24.105 | 1.00 | 29.90 |
| | ATOM | 1428 | C | LEU | 486 | 9.597 | 18.348 | 23.256 | 1.00 | 34.87 |
| | ATOM | 1429 | O | LEU | 486 | 9.078 | 18.225 | 24.362 | 1.00 | 35.85 |
| | ATOM | 1430 | N | ILE | 487 | 9.513 | 19.469 | 22.548 | 1.00 | 35.59 |
| | ATOM | 1431 | CA | ILE | 487 | 8.787 | 20.625 | 23.064 | 1.00 | 36.79 |
| 25 | ATOM | 1432 | CB | ILE | 487 | 8.890 | 21.826 | 22.095 | 1.00 | 37.32 |
| | ATOM | 1433 | CG2 | ILE | 487 | 7.833 | 22.884 | 22.443 | 1.00 | 40.19 |
| | ATOM | 1434 | CG1 | ILE | 487 | 10.292 | 22.443 | 22.181 | 1.00 | 36.00 |
| | ATOM | 1435 | CD1 | ILE | 487 | 10.635 | 23.041 | 23.544 | 1.00 | 33.58 |
| | ATOM | 1436 | C | ILE | 487 | 7.315 | 20.257 | 23.276 | 1.00 | 38.56 |
| 30 | ATOM | 1437 | O | ILE | 487 | 6.708 | 20.628 | 24.282 | 1.00 | 38.52 |
| | ATOM | 1438 | N | HIS | 488 | 6.749 | 19.521 | 22.326 | 1.00 | 40.33 |
| | ATOM | 1439 | CA | HIS | 488 | 5.357 | 19.096 | 22.427 | 1.00 | 42.29 |
| | ATOM | 1440 | CB | HIS | 488 | 4.962 | 18.282 | 21.197 | 1.00 | 44.26 |
| | ATOM | 1441 | CG | HIS | 488 | 3.612 | 17.647 | 21.305 | 1.00 | 47.75 |
| 35 | ATOM | 1442 | CD2 | HIS | 488 | 2.369 | 18.175 | 21.214 | 1.00 | 47.46 |
| | ATOM | 1443 | ND1 | HIS | 488 | 3.440 | 16.298 | 21.534 | 1.00 | 51.09 |
| | ATOM | 1444 | CE1 | HIS | 488 | 2.148 | 16.023 | 21.577 | 1.00 | 51.15 |
| | ATOM | 1445 | NE2 | HIS | 488 | 1.477 | 17.144 | 21.385 | 1.00 | 50.22 |
| | ATOM | 1446 | C | HIS | 488 | 5.154 | 18.254 | 23.685 | 1.00 | 42.55 |
| 40 | ATOM | 1447 | O | HIS | 488 | 4.233 | 18.498 | 24.467 | 1.00 | 43.02 |
| | ATOM | 1448 | N | LEU | 489 | 6.022 | 17.266 | 23.879 | 1.00 | 39.91 |
| | ATOM | 1449 | CA | LEU | 489 | 5.936 | 16.399 | 25.048 | 1.00 | 39.93 |
| | ATOM | 1450 | CB | LEU | 489 | 7.087 | 15.396 | 25.048 | 1.00 | 38.83 |
| | ATOM | 1451 | CG | LEU | 489 | 6.961 | 14.242 | 24.056 | 1.00 | 39.31 |
| 45 | ATOM | 1452 | CD1 | LEU | 489 | 8.259 | 13.456 | 24.027 | 1.00 | 39.01 |
| | ATOM | 1453 | CD2 | LEU | 489 | 5.799 | 13.345 | 24.459 | 1.00 | 41.98 |
| | ATOM | 1454 | C | LEU | 489 | 5.973 | 17.203 | 26.339 | 1.00 | 40.24 |
| | ATOM | 1455 | O | LEU | 489 | 5.267 | 16.888 | 27.298 | 1.00 | 38.72 |
| | ATOM | 1456 | N | MET | 490 | 6.798 | 18.246 | 26.353 | 1.00 | 39.94 |
| 50 | ATOM | 1457 | CA | MET | 490 | 6.939 | 19.102 | 27.522 | 1.00 | 41.50 |
| | ATOM | 1458 | CB | MET | 490 | 8.208 | 19.953 | 27.394 | 1.00 | 39.15 |
| | ATOM | 1459 | CG | MET | 490 | 9.495 | 19.169 | 27.608 | 1.00 | 41.69 |
| | ATOM | 1460 | SD | MET | 490 | 10.978 | 20.106 | 27.161 | 1.00 | 35.76 |
| | ATOM | 1461 | CE | MET | 490 | 12.178 | 18.775 | 27.056 | 1.00 | 39.22 |
| 55 | ATOM | 1462 | C | MET | 490 | 5.718 | 20.004 | 27.717 | 1.00 | 42.33 |
| | ATOM | 1463 | O | MET | 490 | 5.296 | 20.258 | 28.848 | 1.00 | 41.09 |
| | ATOM | 1464 | N | ALA | 491 | 5.162 | 20.498 | 26.616 | 1.00 | 43.15 |
| | ATOM | 1465 | CA | ALA | 491 | 3.983 | 21.351 | 26.693 | 1.00 | 43.79 |
| | ATOM | 1466 | CB | ALA | 491 | 3.622 | 21.879 | 25.311 | 1.00 | 43.93 |
| 60 | ATOM | 1467 | C | ALA | 491 | 2.841 | 20.510 | 27.251 | 1.00 | 46.16 |
| | ATOM | 1468 | O | ALA | 491 | 2.073 | 20.967 | 28.095 | 1.00 | 44.69 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1469 | N | LYS | 492 | 2.752 | 19.268 | 26.783 | 1.00 | 46.29 |
| | ATOM | 1470 | CA | LYS | 492 | 1.711 | 18.351 | 27.222 | 1.00 | 49.90 |
| | ATOM | 1471 | CB | LYS | 492 | 1.772 | 17.053 | 26.411 | 1.00 | 50.03 |
| | ATOM | 1472 | CG | LYS | 492 | 1.087 | 17.135 | 25.062 | 1.00 | 53.81 |
| | ATOM | 1473 | CD | LYS | 492 | -0.002 | 16.084 | 24.930 | 1.00 | 59.00 |
| 10 | ATOM | 1474 | CE | LYS | 492 | -0.988 | 16.453 | 23.827 | 1.00 | 61.85 |
| | ATOM | 1475 | NZ | LYS | 492 | -1.351 | 15.281 | 22.976 | 1.00 | 62.89 |
| | ATOM | 1476 | C | LYS | 492 | 1.841 | 18.025 | 28.701 | 1.00 | 51.15 |
| | ATOM | 1477 | O | LYS | 492 | 0.845 | 17.784 | 29.379 | 1.00 | 53.37 |
| | ATOM | 1478 | N | ALA | 493 | 3.072 | 18.012 | 29.199 | 1.00 | 50.15 |
| 15 | ATOM | 1479 | CA | ALA | 493 | 3.321 | 17.706 | 30.600 | 1.00 | 49.17 |
| | ATOM | 1480 | CB | ALA | 493 | 4.777 | 17.314 | 30.794 | 1.00 | 50.39 |
| | ATOM | 1481 | C | ALA | 493 | 2.971 | 18.885 | 31.501 | 1.00 | 49.36 |
| | ATOM | 1482 | O | ALA | 493 | 3.089 | 18.799 | 32.723 | 1.00 | 51.57 |
| | ATOM | 1483 | N | GLY | 494 | 2.554 | 19.989 | 30.893 | 1.00 | 48.61 |
| 20 | ATOM | 1484 | CA | GLY | 494 | 2.185 | 21.159 | 31.671 | 1.00 | 46.92 |
| | ATOM | 1485 | C | GLY | 494 | 3.322 | 22.107 | 32.006 | 1.00 | 45.46 |
| | ATOM | 1486 | O | GLY | 494 | 3.206 | 22.921 | 32.919 | 1.00 | 43.58 |
| | ATOM | 1487 | N | LEU | 495 | 4.431 | 22.009 | 31.284 | 1.00 | 44.81 |
| | ATOM | 1488 | CA | LEU | 495 | 5.555 | 22.899 | 31.540 | 1.00 | 42.34 |
| 25 | ATOM | 1489 | CB | LEU | 495 | 6.847 | 22.293 | 30.988 | 1.00 | 43.79 |
| | ATOM | 1490 | CG | LEU | 495 | 7.712 | 21.459 | 31.936 | 1.00 | 40.99 |
| | ATOM | 1491 | CD1 | LEU | 495 | 7.022 | 20.156 | 32.260 | 1.00 | 44.70 |
| | ATOM | 1492 | CD2 | LEU | 495 | 9.072 | 21.189 | 31.270 | 1.00 | 42.12 |
| | ATOM | 1493 | C | LEU | 495 | 5.278 | 24.227 | 30.847 | 1.00 | 42.13 |
| 30 | ATOM | 1494 | O | LEU | 495 | 4.664 | 24.258 | 29.778 | 1.00 | 42.49 |
| | ATOM | 1495 | N | THR | 496 | 5.718 | 25.324 | 31.452 | 1.00 | 42.73 |
| | ATOM | 1496 | CA | THR | 496 | 5.521 | 26.636 | 30.845 | 1.00 | 43.56 |
| | ATOM | 1497 | CB | THR | 496 | 5.841 | 27.767 | 31.829 | 1.00 | 46.09 |
| | ATOM | 1498 | OG1 | THR | 496 | 7.222 | 27.688 | 32.208 | 1.00 | 43.92 |
| 35 | ATOM | 1499 | CG2 | THR | 496 | 4.965 | 27.662 | 33.064 | 1.00 | 45.63 |
| | ATOM | 1500 | C | THR | 496 | 6.471 | 26.764 | 29.660 | 1.00 | 45.54 |
| | ATOM | 1501 | O | THR | 496 | 7.370 | 25.939 | 29.488 | 1.00 | 43.39 |
| | ATOM | 1502 | N | LEU | 497 | 6.280 | 27.800 | 28.849 | 1.00 | 45.02 |
| | ATOM | 1503 | CA | LEU | 497 | 7.135 | 28.020 | 27.688 | 1.00 | 45.12 |
| 40 | ATOM | 1504 | CB | LEU | 497 | 6.710 | 29.286 | 26.944 | 1.00 | 46.62 |
| | ATOM | 1505 | CG | LEU | 497 | 5.933 | 29.080 | 25.640 | 1.00 | 50.20 |
| | ATOM | 1506 | CD1 | LEU | 497 | 5.886 | 30.397 | 24.875 | 1.00 | 50.95 |
| | ATOM | 1507 | CD2 | LEU | 497 | 6.589 | 27.990 | 24.798 | 1.00 | 50.91 |
| | ATOM | 1508 | C | LEU | 497 | 8.599 | 28.135 | 28.101 | 1.00 | 44.94 |
| 45 | ATOM | 1509 | O | LEU | 497 | 9.474 | 27.516 | 27.493 | 1.00 | 45.03 |
| | ATOM | 1510 | N | GLN | 498 | 8.862 | 28.927 | 29.137 | 1.00 | 41.14 |
| | ATOM | 1511 | CA | GLN | 498 | 10.221 | 29.101 | 29.627 | 1.00 | 40.54 |
| | ATOM | 1512 | CB | GLN | 498 | 10.246 | 30.140 | 30.743 | 1.00 | 43.82 |
| | ATOM | 1513 | CG | GLN | 498 | 11.585 | 30.270 | 31.437 | 1.00 | 43.37 |
| 50 | ATOM | 1514 | CD | GLN | 498 | 11.539 | 31.260 | 32.584 | 1.00 | 47.03 |
| | ATOM | 1515 | OE1 | GLN | 498 | 10.565 | 31.308 | 33.332 | 1.00 | 49.18 |
| | ATOM | 1516 | NE2 | GLN | 498 | 12.591 | 32.054 | 32.727 | 1.00 | 45.30 |
| | ATOM | 1517 | C | GLN | 498 | 10.777 | 27.773 | 30.145 | 1.00 | 39.39 |
| | ATOM | 1518 | O | GLN | 498 | 11.923 | 27.422 | 29.866 | 1.00 | 35.05 |
| 55 | ATOM | 1519 | N | GLN | 499 | 9.965 | 27.040 | 30.902 | 1.00 | 36.49 |
| | ATOM | 1520 | CA | GLN | 499 | 10.391 | 25.748 | 31.434 | 1.00 | 36.91 |
| | ATOM | 1521 | CB | GLN | 499 | 9.314 | 25.155 | 32.344 | 1.00 | 38.84 |
| | ATOM | 1522 | CG | GLN | 499 | 9.155 | 25.825 | 33.703 | 1.00 | 41.33 |
| | ATOM | 1523 | CD | GLN | 499 | 8.039 | 25.187 | 34.512 | 1.00 | 42.74 |
| 60 | ATOM | 1524 | OE1 | GLN | 499 | 7.027 | 24.760 | 33.955 | 1.00 | 45.44 |
| | ATOM | 1525 | NE2 | GLN | 499 | 8.222 | 25.107 | 35.829 | 1.00 | 43.48 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|-----|
| 5 | ATOM | 1526 | C | GLN | 499 | 10.655 | 24.773 | 30.285 | 1.00 | 35.03 | --- |
| | ATOM | 1527 | O | GLN | 499 | 11.446 | 23.832 | 30.422 | 1.00 | 36.59 | |
| | ATOM | 1528 | N | GLN | 500 | 9.980 | 24.994 | 29.162 | 1.00 | 34.14 | |
| | ATOM | 1529 | CA | GLN | 500 | 10.136 | 24.138 | 27.990 | 1.00 | 34.65 | |
| | ATOM | 1530 | CB | GLN | 500 | 9.042 | 24.436 | 26.958 | 1.00 | 33.90 | |
| 10 | ATOM | 1531 | CG | GLN | 500 | 7.672 | 23.872 | 27.315 | 1.00 | 36.62 | |
| | ATOM | 1532 | CD | GLN | 500 | 6.558 | 24.419 | 26.435 | 1.00 | 40.17 | |
| | ATOM | 1533 | OE1 | GLN | 500 | 6.660 | 24.417 | 25.207 | 1.00 | 40.22 | |
| | ATOM | 1534 | NE2 | GLN | 500 | 5.482 | 24.886 | 27.064 | 1.00 | 41.82 | |
| | ATOM | 1535 | C | GLN | 500 | 11.511 | 24.350 | 27.358 | 1.00 | 34.96 | |
| 15 | ATOM | 1536 | O | GLN | 500 | 12.256 | 23.387 | 27.124 | 1.00 | 30.79 | |
| | ATOM | 1537 | N | HIS | 501 | 11.835 | 25.612 | 27.078 | 1.00 | 34.21 | |
| | ATOM | 1538 | CA | HIS | 501 | 13.117 | 25.966 | 26.480 | 1.00 | 37.42 | |
| | ATOM | 1539 | CB | HIS | 501 | 13.195 | 27.476 | 26.246 | 1.00 | 43.08 | |
| | ATOM | 1540 | CG | HIS | 501 | 12.043 | 28.027 | 25.468 | 1.00 | 51.13 | |
| 20 | ATOM | 1541 | CD2 | HIS | 501 | 11.534 | 27.678 | 24.263 | 1.00 | 53.05 | |
| | ATOM | 1542 | ND1 | HIS | 501 | 11.264 | 29.068 | 25.926 | 1.00 | 54.54 | |
| | ATOM | 1543 | CE1 | HIS | 501 | 10.325 | 29.337 | 25.037 | 1.00 | 54.36 | |
| | ATOM | 1544 | NE2 | HIS | 501 | 10.466 | 28.508 | 24.018 | 1.00 | 55.19 | |
| | ATOM | 1545 | C | HIS | 501 | 14.255 | 25.543 | 27.395 | 1.00 | 35.79 | |
| 25 | ATOM | 1546 | O | HIS | 501 | 15.271 | 24.996 | 26.945 | 1.00 | 36.20 | |
| | ATOM | 1547 | N | GLN | 502 | 14.086 | 25.799 | 28.685 | 1.00 | 33.90 | |
| | ATOM | 1548 | CA | GLN | 502 | 15.110 | 25.438 | 29.650 | 1.00 | 32.18 | |
| | ATOM | 1549 | CB | GLN | 502 | 14.740 | 25.977 | 31.033 | 1.00 | 35.84 | |
| | ATOM | 1550 | CG | GLN | 502 | 14.787 | 27.498 | 31.113 | 1.00 | 32.66 | |
| 30 | ATOM | 1551 | CD | GLN | 502 | 14.420 | 28.028 | 32.486 | 1.00 | 36.62 | |
| | ATOM | 1552 | OE1 | GLN | 502 | 14.102 | 27.262 | 33.397 | 1.00 | 33.99 | |
| | ATOM | 1553 | NE2 | GLN | 502 | 14.462 | 29.348 | 32.640 | 1.00 | 36.22 | |
| | ATOM | 1554 | C | GLN | 502 | 15.340 | 23.932 | 29.716 | 1.00 | 31.79 | |
| | ATOM | 1555 | O | GLN | 502 | 16.483 | 23.479 | 29.769 | 1.00 | 28.00 | |
| 35 | ATOM | 1556 | N | ARG | 503 | 14.266 | 23.146 | 29.705 | 1.00 | 30.99 | |
| | ATOM | 1557 | CA | ARG | 503 | 14.436 | 21.704 | 29.779 | 1.00 | 29.91 | |
| | ATOM | 1558 | CB | ARG | 503 | 13.107 | 21.011 | 30.052 | 1.00 | 32.79 | |
| | ATOM | 1559 | CG | ARG | 503 | 13.258 | 19.541 | 30.400 | 1.00 | 30.84 | |
| | ATOM | 1560 | CD | ARG | 503 | 11.930 | 18.935 | 30.798 | 1.00 | 30.61 | |
| 40 | ATOM | 1561 | NE | ARG | 503 | 12.021 | 17.490 | 30.992 | 1.00 | 28.50 | |
| | ATOM | 1562 | CZ | ARG | 503 | 12.489 | 16.908 | 32.093 | 1.00 | 29.00 | |
| | ATOM | 1563 | NH1 | ARG | 503 | 12.917 | 17.640 | 33.114 | 1.00 | 29.85 | |
| | ATOM | 1564 | NH2 | ARG | 503 | 12.512 | 15.583 | 32.180 | 1.00 | 33.73 | |
| | ATOM | 1565 | C | ARG | 503 | 15.051 | 21.152 | 28.496 | 1.00 | 29.89 | |
| 45 | ATOM | 1566 | O | ARG | 503 | 15.895 | 20.259 | 28.548 | 1.00 | 29.69 | |
| | ATOM | 1567 | N | LEU | 504 | 14.624 | 21.675 | 27.351 | 1.00 | 28.99 | |
| | ATOM | 1568 | CA | LEU | 504 | 15.164 | 21.223 | 26.075 | 1.00 | 28.90 | |
| | ATOM | 1569 | CB | LEU | 504 | 14.566 | 22.023 | 24.916 | 1.00 | 27.72 | |
| | ATOM | 1570 | CG | LEU | 504 | 15.327 | 21.901 | 23.593 | 1.00 | 30.47 | |
| 50 | ATOM | 1571 | CD1 | LEU | 504 | 15.252 | 20.453 | 23.117 | 1.00 | 31.74 | |
| | ATOM | 1572 | CD2 | LEU | 504 | 14.742 | 22.843 | 22.542 | 1.00 | 29.85 | |
| | ATOM | 1573 | C | LEU | 504 | 16.681 | 21.419 | 26.089 | 1.00 | 29.69 | |
| | ATOM | 1574 | O | LEU | 504 | 17.439 | 20.536 | 25.672 | 1.00 | 26.38 | |
| | ATOM | 1575 | N | ALA | 505 | 17.114 | 22.585 | 26.564 | 1.00 | 28.51 | |
| 55 | ATOM | 1576 | CA | ALA | 505 | 18.535 | 22.899 | 26.632 | 1.00 | 25.98 | |
| | ATOM | 1577 | CB | ALA | 505 | 18.735 | 24.361 | 27.039 | 1.00 | 29.86 | |
| | ATOM | 1578 | C | ALA | 505 | 19.261 | 21.977 | 27.604 | 1.00 | 26.67 | |
| | ATOM | 1579 | O | ALA | 505 | 20.340 | 21.462 | 27.290 | 1.00 | 25.54 | |
| | ATOM | 1580 | N | GLN | 506 | 18.677 | 21.771 | 28.784 | 1.00 | 23.59 | |
| 60 | ATOM | 1581 | CA | GLN | 506 | 19.299 | 20.907 | 29.785 | 1.00 | 27.67 | |
| | ATOM | 1582 | CB | GLN | 506 | 18.434 | 20.796 | 31.043 | 1.00 | 27.75 | |

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|----|------|------|-----|------|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1583 | CG | GLN | 506 | 18.414 | 22.027 | 31.945 | 1.00 | 32.48 |
| | ATOM | 1584 | CD | GLN | 506 | 17.111 | 22.116 | 32.736 | 1.00 | 38.40 |
| | ATOM | 1585 | OE1 | GLN | 506 | 16.319 | 21.167 | 32.754 | 1.00 | 35.97 |
| | ATOM | 1586 | NE2 | GLN | 506 | 16.879 | 23.257 | 33.386 | 1.00 | 38.07 |
| | ATOM | 1587 | C | GLN | 506 | 19.500 | 19.509 | 29.217 | 1.00 | 24.53 |
| 10 | ATOM | 1588 | O | GLN | 506 | 20.536 | 18.889 | 29.441 | 1.00 | 26.42 |
| | ATOM | 1589 | N | LEU | 507 | 18.505 | 19.017 | 28.484 | 1.00 | 26.78 |
| | ATOM | 1590 | CA | LEU | 507 | 18.578 | 17.678 | 27.902 | 1.00 | 26.18 |
| | ATOM | 1591 | CB | LEU | 507 | 17.225 | 17.286 | 27.295 | 1.00 | 31.48 |
| | ATOM | 1592 | CG | LEU | 507 | 16.052 | 16.961 | 28.231 | 1.00 | 32.59 |
| 15 | ATOM | 1593 | CD1 | LEU | 507 | 14.836 | 16.561 | 27.389 | 1.00 | 33.78 |
| | ATOM | 1594 | CD2 | LEU | 507 | 16.431 | 15.838 | 29.174 | 1.00 | 30.18 |
| | ATOM | 1595 | C | LEU | 507 | 19.652 | 17.583 | 26.819 | 1.00 | 26.03 |
| | ATOM | 1596 | O | LEU | 507 | 20.421 | 16.621 | 26.771 | 1.00 | 27.28 |
| | ATOM | 1597 | N | LEU | 508 | 19.713 | 18.583 | 25.950 | 1.00 | 24.31 |
| 20 | ATOM | 1598 | CA | LEU | 508 | 20.690 | 18.557 | 24.863 | 1.00 | 23.68 |
| | ATOM | 1599 | CB | LEU | 508 | 20.339 | 19.629 | 23.828 | 1.00 | 23.91 |
| | ATOM | 1600 | CG | LEU | 508 | 19.004 | 19.436 | 23.102 | 1.00 | 24.68 |
| | ATOM | 1601 | CD1 | LEU | 508 | 18.905 | 20.416 | 21.945 | 1.00 | 25.11 |
| | ATOM | 1602 | CD2 | LEU | 508 | 18.903 | 17.994 | 22.580 | 1.00 | 27.53 |
| 25 | ATOM | 1603 | C | LEU | 508 | 22.127 | 18.727 | 25.341 | 1.00 | 22.93 |
| | ATOM | 1604 | O | LEU | 508 | 23.062 | 18.200 | 24.736 | 1.00 | 21.36 |
| | ATOM | 1605 | N | LEU | 509 | 22.302 | 19.451 | 26.441 | 1.00 | 23.86 |
| | ATOM | 1606 | CA | LEU | 509 | 23.637 | 19.661 | 26.991 | 1.00 | 26.28 |
| | ATOM | 1607 | CB | LEU | 509 | 23.598 | 20.735 | 28.095 | 1.00 | 28.08 |
| 30 | ATOM | 1608 | CG | LEU | 509 | 23.578 | 22.214 | 27.672 | 1.00 | 33.98 |
| | ATOM | 1609 | CD1 | LEU | 509 | 23.529 | 23.114 | 28.921 | 1.00 | 35.23 |
| | ATOM | 1610 | CD2 | LEU | 509 | 24.818 | 22.525 | 26.856 | 1.00 | 30.48 |
| | ATOM | 1611 | C | LEU | 509 | 24.154 | 18.327 | 27.540 | 1.00 | 26.08 |
| | ATOM | 1612 | O | LEU | 509 | 25.354 | 18.068 | 27.547 | 1.00 | 23.92 |
| 35 | ATOM | 1613 | N | ILE | 510 | 23.254 | 17.462 | 27.993 | 1.00 | 24.60 |
| | ATOM | 1614 | CA | ILE | 510 | 23.712 | 16.172 | 28.496 | 1.00 | 25.12 |
| | ATOM | 1615 | CB | ILE | 510 | 22.568 | 15.368 | 29.161 | 1.00 | 28.51 |
| | ATOM | 1616 | CG2 | ILE | 510 | 23.051 | 13.965 | 29.506 | 1.00 | 31.67 |
| | ATOM | 1617 | CG1 | ILE | 510 | 22.141 | 16.060 | 30.459 | 1.00 | 31.18 |
| 40 | ATOM | 1618 | CD1 | ILE | 510 | 20.712 | 15.749 | 30.882 | 1.00 | 37.16 |
| | ATOM | 1619 | C | ILE | 510 | 24.337 | 15.351 | 27.364 | 1.00 | 23.86 |
| | ATOM | 1620 | O | ILE | 510 | 25.225 | 14.534 | 27.600 | 1.00 | 24.14 |
| | ATOM | 1621 | N | LEU | 511 | 23.889 | 15.586 | 26.133 | 1.00 | 25.10 |
| | ATOM | 1622 | CA | LEU | 511 | 24.420 | 14.862 | 24.977 | 1.00 | 25.63 |
| 45 | ATOM | 1623 | CB | LEU | 511 | 23.628 | 15.225 | 23.714 | 1.00 | 23.89 |
| | ATOM | 1624 | CG | LEU | 511 | 22.152 | 14.801 | 23.659 | 1.00 | 25.78 |
| | ATOM | 1625 | CD1 | LEU | 511 | 21.648 | 14.920 | 22.224 | 1.00 | 26.55 |
| | ATOM | 1626 | CD2 | LEU | 511 | 21.990 | 13.363 | 24.146 | 1.00 | 26.29 |
| | ATOM | 1627 | C | LEU | 511 | 25.912 | 15.152 | 24.771 | 1.00 | 27.10 |
| 50 | ATOM | 1628 | O | LEU | 511 | 26.641 | 14.332 | 24.214 | 1.00 | 24.98 |
| | ATOM | 1629 | N | SER | 512 | 26.372 | 16.319 | 25.213 | 1.00 | 24.75 |
| | ATOM | 1630 | CA | SER | 512 | 27.787 | 16.637 | 25.076 | 1.00 | 23.68 |
| | ATOM | 1631 | CB | SER | 512 | 28.023 | 18.129 | 25.358 | 1.00 | 26.12 |
| | ATOM | 1632 | OG | SER | 512 | 29.271 | 18.327 | 25.986 | 1.00 | 37.17 |
| 55 | ATOM | 1633 | C | SER | 512 | 28.594 | 15.765 | 26.050 | 1.00 | 23.15 |
| | ATOM | 1634 | O | SER | 512 | 29.742 | 15.383 | 25.769 | 1.00 | 22.15 |
| | ATOM | 1635 | N | AHIS | 513 | 27.993 | 15.456 | 27.192 | 0.50 | 21.53 |
| | ATOM | 1636 | N | BHIS | 513 | 28.008 | 15.453 | 27.202 | 0.50 | 20.99 |
| | ATOM | 1637 | CA | AHIS | 513 | 28.645 | 14.624 | 28.196 | 0.50 | 21.79 |
| 60 | ATOM | 1638 | CA | BHIS | 513 | 28.696 | 14.607 | 28.174 | 0.50 | 20.94 |
| | ATOM | 1639 | CB | AHIS | 513 | 27.920 | 14.776 | 29.536 | 0.50 | 23.59 |

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|----|------|------|-----|------|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1640 | CB | BHIS | 513 | 27.991 | 14.636 | 29.536 | 0.50 | 21.59 |
| | ATOM | 1641 | CG | AHIS | 513 | 28.145 | 16.109 | 30.179 | 0.50 | 27.34 |
| | ATOM | 1642 | CG | BHIS | 513 | 28.800 | 14.032 | 30.642 | 0.50 | 23.94 |
| | ATOM | 1643 | CD2 | AHIS | 513 | 29.223 | 16.616 | 30.824 | 0.50 | 27.56 |
| | ATOM | 1644 | CD2 | BHIS | 513 | 30.095 | 14.211 | 31.001 | 0.50 | 24.22 |
| 10 | ATOM | 1645 | ND1 | AHIS | 513 | 27.204 | 17.117 | 30.160 | 0.50 | 30.62 |
| | ATOM | 1646 | ND1 | BHIS | 513 | 28.285 | 13.105 | 31.523 | 0.50 | 27.00 |
| | ATOM | 1647 | CE1 | AHIS | 513 | 27.693 | 18.185 | 30.763 | 0.50 | 26.32 |
| | ATOM | 1648 | CE1 | BHIS | 513 | 29.225 | 12.740 | 32.376 | 0.50 | 24.40 |
| | ATOM | 1649 | NE2 | AHIS | 513 | 28.916 | 17.908 | 31.176 | 0.50 | 28.30 |
| 15 | ATOM | 1650 | NE2 | BHIS | 513 | 30.334 | 13.396 | 32.081 | 0.50 | 25.54 |
| | ATOM | 1651 | C | AHIS | 513 | 28.666 | 13.164 | 27.738 | 0.50 | 19.81 |
| | ATOM | 1652 | C | BHIS | 513 | 28.720 | 13.171 | 27.652 | 0.50 | 19.42 |
| | ATOM | 1653 | O | AHIS | 513 | 29.601 | 12.426 | 28.026 | 0.50 | 22.45 |
| | ATOM | 1654 | O | BHIS | 513 | 29.707 | 12.457 | 27.809 | 0.50 | 22.62 |
| 20 | ATOM | 1655 | N | ILE | 514 | 27.633 | 12.753 | 27.015 | 1.00 | 20.76 |
| | ATOM | 1656 | CA | ILE | 514 | 27.572 | 11.396 | 26.492 | 1.00 | 20.94 |
| | ATOM | 1657 | CB | ILE | 514 | 26.154 | 11.086 | 25.953 | 1.00 | 27.76 |
| | ATOM | 1658 | CG2 | ILE | 514 | 26.169 | 9.800 | 25.123 | 1.00 | 28.26 |
| | ATOM | 1659 | CG1 | ILE | 514 | 25.185 | 10.965 | 27.139 | 1.00 | 27.91 |
| 25 | ATOM | 1660 | CD1 | ILE | 514 | 23.752 | 10.649 | 26.753 | 1.00 | 34.31 |
| | ATOM | 1661 | C | ILE | 514 | 28.641 | 11.256 | 25.398 | 1.00 | 20.66 |
| | ATOM | 1662 | O | ILE | 514 | 29.298 | 10.226 | 25.285 | 1.00 | 22.21 |
| | ATOM | 1663 | N | ARG | 515 | 28.825 | 12.294 | 24.589 | 1.00 | 20.48 |
| | ATOM | 1664 | CA | ARG | 515 | 29.861 | 12.243 | 23.554 | 1.00 | 21.98 |
| 30 | ATOM | 1665 | CB | ARG | 515 | 29.861 | 13.535 | 22.726 | 1.00 | 23.11 |
| | ATOM | 1666 | CG | ARG | 515 | 31.003 | 13.611 | 21.737 | 1.00 | 25.76 |
| | ATOM | 1667 | CD | ARG | 515 | 30.664 | 12.818 | 20.491 | 1.00 | 28.55 |
| | ATOM | 1668 | NE | ARG | 515 | 29.580 | 13.482 | 19.788 | 1.00 | 36.24 |
| | ATOM | 1669 | CZ | ARG | 515 | 29.615 | 13.827 | 18.508 | 1.00 | 38.91 |
| 35 | ATOM | 1670 | NH1 | ARG | 515 | 30.689 | 13.566 | 17.776 | 1.00 | 35.37 |
| | ATOM | 1671 | NH2 | ARG | 515 | 28.579 | 14.459 | 17.971 | 1.00 | 40.27 |
| | ATOM | 1672 | C | ARG | 515 | 31.221 | 12.087 | 24.225 | 1.00 | 21.29 |
| | ATOM | 1673 | O | ARG | 515 | 32.068 | 11.305 | 23.795 | 1.00 | 20.06 |
| | ATOM | 1674 | N | HIS | 516 | 31.420 | 12.844 | 25.293 | 1.00 | 23.23 |
| 40 | ATOM | 1675 | CA | HIS | 516 | 32.675 | 12.812 | 26.034 | 1.00 | 24.75 |
| | ATOM | 1676 | CB | HIS | 516 | 32.566 | 13.794 | 27.206 | 1.00 | 24.03 |
| | ATOM | 1677 | CG | HIS | 516 | 33.826 | 13.948 | 27.990 | 1.00 | 31.42 |
| | ATOM | 1678 | CD2 | HIS | 516 | 34.138 | 13.587 | 29.257 | 1.00 | 35.87 |
| | ATOM | 1679 | ND1 | HIS | 516 | 34.938 | 14.586 | 27.489 | 1.00 | 33.59 |
| 45 | ATOM | 1680 | CE1 | HIS | 516 | 35.882 | 14.613 | 28.411 | 1.00 | 35.70 |
| | ATOM | 1681 | NE2 | HIS | 516 | 35.422 | 14.013 | 29.495 | 1.00 | 33.35 |
| | ATOM | 1682 | C | HIS | 516 | 32.965 | 11.390 | 26.537 | 1.00 | 24.02 |
| | ATOM | 1683 | O | HIS | 516 | 34.059 | 10.852 | 26.362 | 1.00 | 23.66 |
| | ATOM | 1684 | N | MET | 517 | 31.969 | 10.786 | 27.168 | 1.00 | 20.91 |
| 50 | ATOM | 1685 | CA | MET | 517 | 32.109 | 9.436 | 27.684 | 1.00 | 24.21 |
| | ATOM | 1686 | CB | MET | 517 | 30.837 | 9.038 | 28.424 | 1.00 | 23.88 |
| | ATOM | 1687 | CG | MET | 517 | 30.607 | 9.903 | 29.652 | 1.00 | 26.32 |
| | ATOM | 1688 | SD | MET | 517 | 29.435 | 9.222 | 30.790 | 1.00 | 26.67 |
| | ATOM | 1689 | CE | MET | 517 | 27.914 | 9.390 | 29.807 | 1.00 | 23.26 |
| 55 | ATOM | 1690 | C | MET | 517 | 32.399 | 8.448 | 26.564 | 1.00 | 23.26 |
| | ATOM | 1691 | O | MET | 517 | 33.213 | 7.547 | 26.728 | 1.00 | 26.08 |
| | ATOM | 1692 | N | SER | 518 | 31.736 | 8.612 | 25.423 | 1.00 | 21.93 |
| | ATOM | 1693 | CA | SER | 518 | 31.977 | 7.717 | 24.301 | 1.00 | 23.08 |
| | ATOM | 1694 | CB | SER | 518 | 30.976 | 8.027 | 23.173 | 1.00 | 22.02 |
| 60 | ATOM | 1695 | OG | SER | 518 | 31.283 | 7.336 | 21.978 | 1.00 | 24.01 |
| | ATOM | 1696 | C | SER | 518 | 33.432 | 7.862 | 23.810 | 1.00 | 25.15 |

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|----|------|------|-----|------|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1697 | O | SER | 518 | 34.111 | 6.866 | 23.532 | 1.00 | 22.94 |
| | ATOM | 1698 | N | ASN | 519 | 33.923 | 9.097 | 23.713 | 1.00 | 22.42 |
| | ATOM | 1699 | CA | ASN | 519 | 35.295 | 9.309 | 23.260 | 1.00 | 21.87 |
| | ATOM | 1700 | CB | ASN | 519 | 35.605 | 10.807 | 23.157 | 1.00 | 24.46 |
| | ATOM | 1701 | CG | ASN | 519 | 34.864 | 11.469 | 22.021 | 1.00 | 29.02 |
| 10 | ATOM | 1702 | OD1 | ASN | 519 | 34.661 | 10.864 | 20.965 | 1.00 | 31.93 |
| | ATOM | 1703 | ND2 | ASN | 519 | 34.459 | 12.715 | 22.224 | 1.00 | 28.81 |
| | ATOM | 1704 | C | ASN | 519 | 36.292 | 8.643 | 24.201 | 1.00 | 21.46 |
| | ATOM | 1705 | O | ASN | 519 | 37.251 | 8.015 | 23.752 | 1.00 | 23.56 |
| | ATOM | 1706 | N | LYS | 520 | 36.070 | 8.782 | 25.504 | 1.00 | 23.23 |
| 15 | ATOM | 1707 | CA | LYS | 520 | 36.964 | 8.171 | 26.488 | 1.00 | 26.35 |
| | ATOM | 1708 | CB | LYS | 520 | 36.581 | 8.592 | 27.912 | 1.00 | 27.53 |
| | ATOM | 1709 | CG | LYS | 520 | 36.618 | 10.101 | 28.174 | 1.00 | 33.74 |
| | ATOM | 1710 | CD | LYS | 520 | 37.962 | 10.710 | 27.811 | 1.00 | 42.09 |
| | ATOM | 1711 | CE | LYS | 520 | 39.047 | 10.307 | 28.802 | 1.00 | 43.97 |
| 20 | ATOM | 1712 | NZ | LYS | 520 | 39.858 | 11.480 | 29.254 | 1.00 | 48.07 |
| | ATOM | 1713 | C | LYS | 520 | 36.899 | 6.644 | 26.376 | 1.00 | 27.71 |
| | ATOM | 1714 | O | LYS | 520 | 37.913 | 5.957 | 26.501 | 1.00 | 27.15 |
| | ATOM | 1715 | N | GLY | 521 | 35.704 | 6.117 | 26.141 | 1.00 | 25.02 |
| | ATOM | 1716 | CA | GLY | 521 | 35.562 | 4.676 | 26.003 | 1.00 | 26.67 |
| 25 | ATOM | 1717 | C | GLY | 521 | 36.254 | 4.168 | 24.753 | 1.00 | 27.06 |
| | ATOM | 1718 | O | GLY | 521 | 36.924 | 3.128 | 24.775 | 1.00 | 26.84 |
| | ATOM | 1719 | N | AMET | 522 | 36.101 | 4.893 | 23.650 | 0.50 | 25.87 |
| | ATOM | 1720 | N | BMET | 522 | 36.095 | 4.908 | 23.658 | 0.50 | 27.62 |
| | ATOM | 1721 | CA | AMET | 522 | 36.727 | 4.491 | 22.401 | 0.50 | 27.27 |
| 30 | ATOM | 1722 | CA | BMET | 522 | 36.703 | 4.551 | 22.384 | 0.50 | 30.14 |
| | ATOM | 1723 | CB | AMET | 522 | 36.267 | 5.396 | 21.260 | 0.50 | 26.50 |
| | ATOM | 1724 | CB | BMET | 522 | 36.252 | 5.525 | 21.288 | 0.50 | 32.46 |
| | ATOM | 1725 | CG | AMET | 522 | 34.827 | 5.162 | 20.866 | 0.50 | 25.05 |
| | ATOM | 1726 | CG | BMET | 522 | 35.681 | 4.854 | 20.045 | 0.50 | 35.70 |
| 35 | ATOM | 1727 | SD | AMET | 522 | 34.585 | 3.587 | 20.020 | 0.50 | 27.07 |
| | ATOM | 1728 | SD | BMET | 522 | 34.197 | 5.672 | 19.408 | 0.50 | 40.01 |
| | ATOM | 1729 | CE | AMET | 522 | 33.142 | 4.017 | 19.031 | 0.50 | 31.29 |
| | ATOM | 1730 | CE | BMET | 522 | 34.733 | 6.085 | 17.745 | 0.50 | 42.12 |
| | ATOM | 1731 | C | AMET | 522 | 38.242 | 4.532 | 22.512 | 0.50 | 28.99 |
| 40 | ATOM | 1732 | C | BMET | 522 | 38.224 | 4.567 | 22.483 | 0.50 | 30.76 |
| | ATOM | 1733 | O | AMET | 522 | 38.939 | 3.743 | 21.870 | 0.50 | 31.65 |
| | ATOM | 1734 | O | BMET | 522 | 38.905 | 3.793 | 21.807 | 0.50 | 32.87 |
| | ATOM | 1735 | N | GLU | 523 | 38.749 | 5.452 | 23.324 | 1.00 | 30.85 |
| | ATOM | 1736 | CA | GLU | 523 | 40.190 | 5.576 | 23.513 | 1.00 | 34.09 |
| 45 | ATOM | 1737 | CB | GLU | 523 | 40.515 | 6.725 | 24.480 | 1.00 | 35.59 |
| | ATOM | 1738 | CG | GLU | 523 | 40.658 | 8.079 | 23.784 | 1.00 | 43.35 |
| | ATOM | 1739 | CD | GLU | 523 | 40.560 | 9.265 | 24.739 | 1.00 | 46.63 |
| | ATOM | 1740 | OE1 | GLU | 523 | 39.832 | 10.240 | 24.416 | 1.00 | 47.64 |
| | ATOM | 1741 | OE2 | GLU | 523 | 41.212 | 9.225 | 25.805 | 1.00 | 43.09 |
| 50 | ATOM | 1742 | C | GLU | 523 | 40.718 | 4.260 | 24.061 | 1.00 | 34.62 |
| | ATOM | 1743 | O | GLU | 523 | 41.733 | 3.747 | 23.596 | 1.00 | 33.87 |
| | ATOM | 1744 | N | HIS | 524 | 40.021 | 3.700 | 25.042 | 1.00 | 36.33 |
| | ATOM | 1745 | CA | HIS | 524 | 40.455 | 2.427 | 25.607 | 1.00 | 39.20 |
| | ATOM | 1746 | CB | HIS | 524 | 39.678 | 2.093 | 26.878 | 1.00 | 40.75 |
| 55 | ATOM | 1747 | CG | HIS | 524 | 40.061 | 0.774 | 27.473 | 1.00 | 48.10 |
| | ATOM | 1748 | CD2 | HIS | 524 | 41.192 | 0.376 | 28.104 | 1.00 | 48.56 |
| | ATOM | 1749 | ND1 | HIS | 524 | 39.247 | -0.338 | 27.412 | 1.00 | 48.84 |
| | ATOM | 1750 | CE1 | HIS | 524 | 39.859 | -1.362 | 27.978 | 1.00 | 50.19 |
| | ATOM | 1751 | NE2 | HIS | 524 | 41.041 | -0.956 | 28.407 | 1.00 | 51.61 |
| 60 | ATOM | 1752 | C | HIS | 524 | 40.290 | 1.282 | 24.613 | 1.00 | 38.06 |
| | ATOM | 1753 | O | HIS | 524 | 41.226 | 0.521 | 24.371 | 1.00 | 38.18 |

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|----|------|------|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 1754 | N | LEU | 525 | 39.101 | 1.162 | 24.034 | 1.00 | 36.96 |
| | ATOM | 1755 | CA | LEU | 525 | 38.831 | 0.093 | 23.084 | 1.00 | 37.40 |
| | ATOM | 1756 | CB | LEU | 525 | 37.416 | 0.241 | 22.514 | 1.00 | 35.89 |
| | ATOM | 1757 | CG | LEU | 525 | 36.268 | 0.107 | 23.527 | 1.00 | 33.17 |
| | ATOM | 1758 | CD1 | LEU | 525 | 34.936 | 0.246 | 22.811 | 1.00 | 31.77 |
| 10 | ATOM | 1759 | CD2 | LEU | 525 | 36.343 | -1.240 | 24.238 | 1.00 | 35.92 |
| | ATOM | 1760 | C | LEU | 525 | 39.859 | 0.057 | 21.954 | 1.00 | 41.32 |
| | ATOM | 1761 | O | LEU | 525 | 40.244 | -1.015 | 21.487 | 1.00 | 40.76 |
| | ATOM | 1762 | N | TYR | 526 | 40.314 | 1.227 | 21.522 | 1.00 | 43.68 |
| | ATOM | 1763 | CA | TYR | 526 | 41.300 | 1.297 | 20.449 | 1.00 | 49.00 |
| 15 | ATOM | 1764 | CB | TYR | 526 | 41.376 | 2.722 | 19.890 | 1.00 | 51.86 |
| | ATOM | 1765 | CG | TYR | 526 | 42.305 | 2.878 | 18.704 | 1.00 | 57.70 |
| | ATOM | 1766 | CD1 | TYR | 526 | 41.835 | 2.718 | 17.400 | 1.00 | 58.93 |
| | ATOM | 1767 | CE1 | TYR | 526 | 42.681 | 2.875 | 16.305 | 1.00 | 61.21 |
| | ATOM | 1768 | CD2 | TYR | 526 | 43.653 | 3.200 | 18.883 | 1.00 | 58.58 |
| 20 | ATOM | 1769 | CE2 | TYR | 526 | 44.510 | 3.359 | 17.790 | 1.00 | 61.15 |
| | ATOM | 1770 | CZ | TYR | 526 | 44.016 | 3.194 | 16.505 | 1.00 | 61.09 |
| | ATOM | 1771 | OH | TYR | 526 | 44.851 | 3.343 | 15.417 | 1.00 | 63.79 |
| | ATOM | 1772 | C | TYR | 526 | 42.671 | 0.871 | 20.964 | 1.00 | 50.14 |
| | ATOM | 1773 | O | TYR | 526 | 43.471 | 0.303 | 20.223 | 1.00 | 50.73 |
| 25 | ATOM | 1774 | N | SER | 527 | 42.930 | 1.139 | 22.240 | 1.00 | 52.72 |
| | ATOM | 1775 | CA | SER | 527 | 44.205 | 0.790 | 22.857 | 1.00 | 55.88 |
| | ATOM | 1776 | CB | SER | 527 | 44.351 | 1.516 | 24.199 | 1.00 | 55.00 |
| | ATOM | 1777 | OG | SER | 527 | 43.752 | 0.788 | 25.257 | 1.00 | 52.46 |
| | ATOM | 1778 | C | SER | 527 | 44.365 | -0.718 | 23.054 | 1.00 | 60.39 |
| 30 | ATOM | 1779 | O | SER | 527 | 45.398 | -1.185 | 23.534 | 1.00 | 60.43 |
| | ATOM | 1780 | N | MET | 528 | 43.335 | -1.472 | 22.678 | 1.00 | 63.86 |
| | ATOM | 1781 | CA | MET | 528 | 43.347 | -2.929 | 22.788 | 1.00 | 67.95 |
| | ATOM | 1782 | CB | MET | 528 | 42.534 | -3.381 | 24.008 | 1.00 | 67.85 |
| | ATOM | 1783 | CG | MET | 528 | 41.237 | -2.606 | 24.222 | 1.00 | 70.10 |
| 35 | ATOM | 1784 | SD | MET | 528 | 39.895 | -3.569 | 24.983 | 1.00 | 71.70 |
| | ATOM | 1785 | CE | MET | 528 | 39.231 | -4.412 | 23.554 | 1.00 | 72.57 |
| | ATOM | 1786 | C | MET | 528 | 42.726 | -3.502 | 21.513 | 1.00 | 70.33 |
| | ATOM | 1787 | O | MET | 528 | 42.170 | -4.602 | 21.513 | 1.00 | 72.43 |
| | ATOM | 1788 | N | LYS | 529 | 42.834 | -2.739 | 20.428 | 1.00 | 71.53 |
| 40 | ATOM | 1789 | CA | LYS | 529 | 42.274 | -3.122 | 19.136 | 1.00 | 72.00 |
| | ATOM | 1790 | CB | LYS | 529 | 42.508 | -2.004 | 18.119 | 1.00 | 71.30 |
| | ATOM | 1791 | C | LYS | 529 | 42.813 | -4.439 | 18.587 | 1.00 | 72.47 |
| | ATOM | 1792 | O | LYS | 529 | 43.990 | -4.762 | 18.751 | 1.00 | 70.37 |
| | ATOM | 1793 | N | CYS | 530 | 41.932 | -5.191 | 17.930 | 1.00 | 74.48 |
| 45 | ATOM | 1794 | CA | CYS | 530 | 42.279 | -6.474 | 17.325 | 1.00 | 76.67 |
| | ATOM | 1795 | CB | CYS | 530 | 41.004 | -7.245 | 16.952 | 1.00 | 77.23 |
| | ATOM | 1796 | SG | CYS | 530 | 40.447 | -8.491 | 18.146 | 1.00 | 79.38 |
| | ATOM | 1797 | C | CYS | 530 | 43.098 | -6.220 | 16.065 | 1.00 | 78.08 |
| | ATOM | 1798 | O | CYS | 530 | 43.241 | -5.076 | 15.623 | 1.00 | 78.81 |
| 50 | ATOM | 1799 | N | LYS | 531 | 43.637 | -7.289 | 15.487 | 1.00 | 78.22 |
| | ATOM | 1800 | CA | LYS | 531 | 44.424 | -7.187 | 14.267 | 1.00 | 78.15 |
| | ATOM | 1801 | CB | LYS | 531 | 45.600 | -8.182 | 14.305 | 1.00 | 78.33 |
| | ATOM | 1802 | C | LYS | 531 | 43.508 | -7.467 | 13.067 | 1.00 | 77.93 |
| | ATOM | 1803 | O | LYS | 531 | 42.549 | -6.734 | 12.839 | 1.00 | 78.07 |
| 55 | ATOM | 1804 | N | ASN | 532 | 43.784 | -8.539 | 12.328 | 1.00 | 77.80 |
| | ATOM | 1805 | CA | ASN | 532 | 42.984 | -8.902 | 11.152 | 1.00 | 77.30 |
| | ATOM | 1806 | CB | ASN | 532 | 43.550 | -10.166 | 10.521 | 1.00 | 77.55 |
| | ATOM | 1807 | C | ASN | 532 | 41.485 | -9.082 | 11.423 | 1.00 | 77.34 |
| | ATOM | 1808 | O | ASN | 532 | 40.904 | -10.123 | 11.118 | 1.00 | 78.13 |
| 60 | ATOM | 1809 | N | VAL | 533 | 40.859 | -8.055 | 11.988 | 1.00 | 76.13 |
| | ATOM | 1810 | CA | VAL | 533 | 39.436 | -8.098 | 12.280 | 1.00 | 73.77 |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| 5 | ATOM | 1811 | CB | VAL | 533 | 39.155 | -7.715 | 13.752 | 1.00 | 73.62 |
| | ATOM | 1812 | CG1 | VAL | 533 | 39.690 | -6.327 | 14.047 | 1.00 | 73.13 |
| | ATOM | 1813 | CG2 | VAL | 533 | 37.662 | -7.782 | 14.021 | 1.00 | 73.14 |
| | ATOM | 1814 | C | VAL | 533 | 38.685 | -7.143 | 11.352 | 1.00 | 72.97 |
| | ATOM | 1815 | O | VAL | 533 | 39.024 | -5.960 | 11.252 | 1.00 | 73.91 |
| 10 | ATOM | 1816 | N | VAL | 534 | 37.671 | -7.666 | 10.666 | 1.00 | 70.02 |
| | ATOM | 1817 | CA | VAL | 534 | 36.866 | -6.867 | 9.747 | 1.00 | 66.70 |
| | ATOM | 1818 | CB | VAL | 534 | 35.619 | -7.646 | 9.328 | 1.00 | 67.32 |
| | ATOM | 1819 | C | VAL | 534 | 36.463 | -5.541 | 10.393 | 1.00 | 63.87 |
| | ATOM | 1820 | O | VAL | 534 | 35.895 | -5.519 | 11.486 | 1.00 | 63.55 |
| 15 | ATOM | 1821 | N | PRO | 535 | 36.756 | -4.415 | 9.719 | 1.00 | 60.92 |
| | ATOM | 1822 | CD | PRO | 535 | 37.424 | -4.354 | 8.408 | 1.00 | 61.01 |
| | ATOM | 1823 | CA | PRO | 535 | 36.424 | -3.077 | 10.229 | 1.00 | 56.83 |
| | ATOM | 1824 | CB | PRO | 535 | 36.867 | -2.135 | 9.107 | 1.00 | 58.70 |
| | ATOM | 1825 | CG | PRO | 535 | 37.023 | -3.009 | 7.893 | 1.00 | 61.55 |
| 20 | ATOM | 1826 | C | PRO | 535 | 34.944 | -2.902 | 10.571 | 1.00 | 52.90 |
| | ATOM | 1827 | O | PRO | 535 | 34.067 | -3.461 | 9.908 | 1.00 | 52.01 |
| | ATOM | 1828 | N | LEU | 536 | 34.672 | -2.120 | 11.610 | 1.00 | 48.60 |
| | ATOM | 1829 | CA | LEU | 536 | 33.301 | -1.874 | 12.042 | 1.00 | 45.08 |
| | ATOM | 1830 | CB | LEU | 536 | 33.280 | -0.796 | 13.128 | 1.00 | 44.35 |
| 25 | ATOM | 1831 | CG | LEU | 536 | 32.267 | -0.911 | 14.273 | 1.00 | 43.48 |
| | ATOM | 1832 | CD1 | LEU | 536 | 31.919 | 0.490 | 14.745 | 1.00 | 43.41 |
| | ATOM | 1833 | CD2 | LEU | 536 | 31.022 | -1.654 | 13.835 | 1.00 | 39.55 |
| | ATOM | 1834 | C | LEU | 536 | 32.434 | -1.433 | 10.871 | 1.00 | 43.58 |
| | ATOM | 1835 | O | LEU | 536 | 31.287 | -1.862 | 10.734 | 1.00 | 42.14 |
| 30 | ATOM | 1836 | N | TYR | 537 | 32.992 | -0.575 | 10.024 | 1.00 | 43.02 |
| | ATOM | 1837 | CA | TYR | 537 | 32.269 | -0.066 | 8.866 | 1.00 | 43.34 |
| | ATOM | 1838 | CB | TYR | 537 | 33.200 | 0.786 | 7.997 | 1.00 | 44.76 |
| | ATOM | 1839 | CG | TYR | 537 | 32.483 | 1.558 | 6.913 | 1.00 | 48.28 |
| | ATOM | 1840 | CD1 | TYR | 537 | 32.190 | 0.964 | 5.687 | 1.00 | 48.46 |
| 35 | ATOM | 1841 | CE1 | TYR | 537 | 31.504 | 1.660 | 4.693 | 1.00 | 52.48 |
| | ATOM | 1842 | CD2 | TYR | 537 | 32.073 | 2.875 | 7.123 | 1.00 | 49.99 |
| | ATOM | 1843 | CE2 | TYR | 537 | 31.383 | 3.584 | 6.135 | 1.00 | 53.73 |
| | ATOM | 1844 | CZ | TYR | 537 | 31.100 | 2.967 | 4.924 | 1.00 | 54.01 |
| | ATOM | 1845 | OH | TYR | 537 | 30.401 | 3.648 | 3.952 | 1.00 | 55.90 |
| 40 | ATOM | 1846 | C | TYR | 537 | 31.683 | -1.199 | 8.032 | 1.00 | 43.15 |
| | ATOM | 1847 | O | TYR | 537 | 30.500 | -1.191 | 7.696 | 1.00 | 41.54 |
| | ATOM | 1848 | N | ASP | 538 | 32.521 | -2.175 | 7.702 | 1.00 | 44.67 |
| | ATOM | 1849 | CA | ASP | 538 | 32.097 | -3.309 | 6.893 | 1.00 | 45.49 |
| | ATOM | 1850 | CB | ASP | 538 | 33.322 | -4.126 | 6.479 | 1.00 | 51.32 |
| 45 | ATOM | 1851 | CG | ASP | 538 | 34.361 | -3.284 | 5.748 | 1.00 | 56.17 |
| | ATOM | 1852 | OD1 | ASP | 538 | 35.436 | -3.820 | 5.396 | 1.00 | 57.29 |
| | ATOM | 1853 | OD2 | ASP | 538 | 34.097 | -2.079 | 5.526 | 1.00 | 59.24 |
| | ATOM | 1854 | C | ASP | 538 | 31.071 | -4.195 | 7.587 | 1.00 | 43.48 |
| | ATOM | 1855 | O | ASP | 538 | 30.177 | -4.738 | 6.940 | 1.00 | 43.95 |
| 50 | ATOM | 1856 | N | LEU | 539 | 31.193 | -4.345 | 8.901 | 1.00 | 41.57 |
| | ATOM | 1857 | CA | LEU | 539 | 30.244 | -5.157 | 9.654 | 1.00 | 39.11 |
| | ATOM | 1858 | CB | LEU | 539 | 30.734 | -5.351 | 11.092 | 1.00 | 41.88 |
| | ATOM | 1859 | CG | LEU | 539 | 29.770 | -6.065 | 12.044 | 1.00 | 46.11 |
| | ATOM | 1860 | CD1 | LEU | 539 | 29.298 | -7.379 | 11.423 | 1.00 | 46.99 |
| 55 | ATOM | 1861 | CD2 | LEU | 539 | 30.474 | -6.319 | 13.377 | 1.00 | 45.76 |
| | ATOM | 1862 | C | LEU | 539 | 28.891 | -4.451 | 9.651 | 1.00 | 36.38 |
| | ATOM | 1863 | O | LEU | 539 | 27.849 | -5.070 | 9.436 | 1.00 | 35.74 |
| | ATOM | 1864 | N | LEU | 540 | 28.919 | -3.146 | 9.894 | 1.00 | 35.50 |
| | ATOM | 1865 | CA | LEU | 540 | 27.703 | -2.336 | 9.903 | 1.00 | 35.59 |
| 60 | ATOM | 1866 | CB | LEU | 540 | 28.061 | -0.877 | 10.219 | 1.00 | 37.63 |
| | ATOM | 1867 | CG | LEU | 540 | 27.856 | -0.252 | 11.605 | 1.00 | 40.28 |

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|----|------|------|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 1868 | CD1 | LEU | 540 | 27.526 | -1.299 | 12.645 | 1.00 | 38.55 |
| | ATOM | 1869 | CD2 | LEU | 540 | 29.114 | 0.506 | 11.985 | 1.00 | 41.04 |
| | ATOM | 1870 | C | LEU | 540 | 27.060 | -2.415 | 8.510 | 1.00 | 35.50 |
| | ATOM | 1871 | O | LEU | 540 | 25.846 | -2.585 | 8.371 | 1.00 | 33.21 |
| | ATOM | 1872 | N | LEU | 541 | 27.892 | -2.289 | 7.483 | 1.00 | 37.01 |
| 10 | ATOM | 1873 | CA | LEU | 541 | 27.418 | -2.340 | 6.101 | 1.00 | 38.51 |
| | ATOM | 1874 | CB | LEU | 541 | 28.591 | -2.152 | 5.145 | 1.00 | 39.67 |
| | ATOM | 1875 | CG | LEU | 541 | 28.301 | -2.112 | 3.643 | 1.00 | 40.92 |
| | ATOM | 1876 | CD1 | LEU | 541 | 27.184 | -1.130 | 3.348 | 1.00 | 42.44 |
| | ATOM | 1877 | CD2 | LEU | 541 | 29.572 | -1.716 | 2.908 | 1.00 | 44.18 |
| 15 | ATOM | 1878 | C | LEU | 541 | 26.723 | -3.676 | 5.833 | 1.00 | 39.75 |
| | ATOM | 1879 | O | LEU | 541 | 25.616 | -3.713 | 5.297 | 1.00 | 36.48 |
| | ATOM | 1880 | N | GLU | 542 | 27.366 | -4.770 | 6.230 | 1.00 | 40.88 |
| | ATOM | 1881 | CA | GLU | 542 | 26.790 | -6.097 | 6.037 | 1.00 | 41.89 |
| | ATOM | 1882 | CB | GLU | 542 | 27.719 | -7.170 | 6.620 | 1.00 | 44.11 |
| 20 | ATOM | 1883 | CG | GLU | 542 | 27.010 | -8.457 | 7.052 | 1.00 | 50.60 |
| | ATOM | 1884 | CD | GLU | 542 | 26.434 | -9.245 | 5.887 | 1.00 | 55.80 |
| | ATOM | 1885 | OE1 | GLU | 542 | 25.570 | -10.117 | 6.130 | 1.00 | 58.81 |
| | ATOM | 1886 | OE2 | GLU | 542 | 26.842 | -8.996 | 4.728 | 1.00 | 57.19 |
| | ATOM | 1887 | C | GLU | 542 | 25.414 | -6.195 | 6.691 | 1.00 | 41.58 |
| 25 | ATOM | 1888 | O | GLU | 542 | 24.472 | -6.720 | 6.102 | 1.00 | 42.82 |
| | ATOM | 1889 | N | MET | 543 | 25.298 | -5.686 | 7.915 | 1.00 | 40.09 |
| | ATOM | 1890 | CA | MET | 543 | 24.036 | -5.731 | 8.634 | 1.00 | 36.43 |
| | ATOM | 1891 | CB | MET | 543 | 24.270 | -5.424 | 10.111 | 1.00 | 39.95 |
| | ATOM | 1892 | CG | MET | 543 | 25.137 | -6.459 | 10.808 | 1.00 | 41.95 |
| 30 | ATOM | 1893 | SD | MET | 543 | 24.918 | -6.445 | 12.604 | 1.00 | 47.17 |
| | ATOM | 1894 | CE | MET | 543 | 25.324 | -4.749 | 12.964 | 1.00 | 40.88 |
| | ATOM | 1895 | C | MET | 543 | 23.001 | -4.769 | 8.072 | 1.00 | 35.02 |
| | ATOM | 1896 | O | MET | 543 | 21.808 | -5.073 | 8.048 | 1.00 | 35.31 |
| | ATOM | 1897 | N | LEU | 544 | 23.457 | -3.605 | 7.629 | 1.00 | 32.90 |
| 35 | ATOM | 1898 | CA | LEU | 544 | 22.559 | -2.603 | 7.074 | 1.00 | 36.88 |
| | ATOM | 1899 | CB | LEU | 544 | 23.225 | -1.226 | 7.111 | 1.00 | 34.51 |
| | ATOM | 1900 | CG | LEU | 544 | 23.268 | -0.562 | 8.490 | 1.00 | 31.94 |
| | ATOM | 1901 | CD1 | LEU | 544 | 24.284 | 0.564 | 8.478 | 1.00 | 32.27 |
| | ATOM | 1902 | CD2 | LEU | 544 | 21.897 | -0.029 | 8.846 | 1.00 | 29.02 |
| 40 | ATOM | 1903 | C | LEU | 544 | 22.148 | -2.941 | 5.640 | 1.00 | 38.94 |
| | ATOM | 1904 | O | LEU | 544 | 20.971 | -2.842 | 5.294 | 1.00 | 39.52 |
| | ATOM | 1905 | N | ASP | 545 | 23.118 | -3.338 | 4.817 | 1.00 | 41.05 |
| | ATOM | 1906 | CA | ASP | 545 | 22.850 | -3.685 | 3.418 | 1.00 | 40.78 |
| | ATOM | 1907 | CB | ASP | 545 | 24.159 | -3.780 | 2.620 | 1.00 | 37.75 |
| 45 | ATOM | 1908 | CG | ASP | 545 | 23.922 | -3.937 | 1.120 | 1.00 | 35.19 |
| | ATOM | 1909 | OD1 | ASP | 545 | 24.881 | -4.265 | 0.380 | 1.00 | 33.48 |
| | ATOM | 1910 | OD2 | ASP | 545 | 22.768 | -3.734 | 0.691 | 1.00 | 31.33 |
| | ATOM | 1911 | C | ASP | 545 | 22.116 | -5.015 | 3.349 | 1.00 | 42.87 |
| | ATOM | 1912 | O | ASP | 545 | 22.681 | -6.030 | 2.929 | 1.00 | 44.32 |
| 50 | ATOM | 1913 | N | ALA | 546 | 20.853 | -5.009 | 3.755 | 1.00 | 43.49 |
| | ATOM | 1914 | CA | ALA | 546 | 20.069 | -6.229 | 3.746 | 1.00 | 46.96 |
| | ATOM | 1915 | CB | ALA | 546 | 19.213 | -6.305 | 5.006 | 1.00 | 47.82 |
| | ATOM | 1916 | C | ALA | 546 | 19.193 | -6.362 | 2.508 | 1.00 | 49.55 |
| | ATOM | 1917 | O | ALA | 546 | 18.804 | -5.368 | 1.883 | 1.00 | 48.75 |
| 55 | ATOM | 1918 | N | HIS | 547 | 18.895 | -7.606 | 2.152 | 1.00 | 50.98 |
| | ATOM | 1919 | CA | HIS | 547 | 18.042 | -7.884 | 1.006 | 1.00 | 53.77 |
| | ATOM | 1920 | CB | HIS | 547 | 18.431 | -9.223 | 0.369 | 1.00 | 52.69 |
| | ATOM | 1921 | CG | HIS | 547 | 18.395 | -10.382 | 1.317 | 1.00 | 55.05 |
| | ATOM | 1922 | CD2 | HIS | 547 | 17.477 | -10.752 | 2.242 | 1.00 | 53.94 |
| 60 | ATOM | 1923 | ND1 | HIS | 547 | 19.395 | -11.329 | 1.371 | 1.00 | 56.23 |
| | ATOM | 1924 | CE1 | HIS | 547 | 19.095 | -12.232 | 2.286 | 1.00 | 55.36 |

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|----|--------|------|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | ATOM | 1925 | NE2 | HIS | 547 | 17.936 | -11.906 | 2.830 | 1.00 | 57.01 |
| | ATOM | 1926 | C | HIS | 547 | 16.603 | -7.936 | 1.518 | 1.00 | 55.69 |
| | ATOM | 1927 | O | HIS | 547 | 16.362 | -7.796 | 2.720 | 1.00 | 54.30 |
| | ATOM | 1928 | N | ARG | 548 | 15.653 | -8.139 | 0.612 | 1.00 | 57.00 |
| | ATOM | 1929 | CA | ARG | 548 | 14.245 | -8.212 | 0.987 | 1.00 | 60.65 |
| 10 | ATOM | 1930 | CB | ARG | 548 | 13.432 | -7.171 | 0.208 | 1.00 | 62.69 |
| | ATOM | 1931 | CG | ARG | 548 | 14.272 | -6.222 | -0.637 | 1.00 | 67.54 |
| | ATOM | 1932 | CD | ARG | 548 | 13.448 | -5.061 | -1.171 | 1.00 | 71.92 |
| | ATOM | 1933 | NE | ARG | 548 | 13.702 | -3.826 | -0.432 | 1.00 | 76.95 |
| | ATOM | 1934 | CZ | ARG | 548 | 14.864 | -3.178 | -0.429 | 1.00 | 79.04 |
| 15 | ATOM | 1935 | NH1 | ARG | 548 | 15.891 | -3.644 | -1.128 | 1.00 | 80.66 |
| | ATOM | 1936 | NH2 | ARG | 548 | 15.001 | -2.063 | 0.278 | 1.00 | 80.39 |
| | ATOM | 1937 | C | ARG | 548 | 13.695 | -9.608 | 0.711 | 1.00 | 61.65 |
| | ATOM | 1938 | O | ARG | 548 | 12.500 | -9.781 | 0.466 | 1.00 | 62.05 |
| | ATOM | 1939 | N | LEU | 549 | 14.576 | -10.603 | 0.756 | 1.00 | 62.39 |
| 20 | ATOM | 1940 | CA | LEU | 549 | 14.188 | -11.985 | 0.507 | 1.00 | 64.02 |
| | ATOM | 1941 | CB | LEU | 549 | 15.433 | -12.828 | 0.195 | 1.00 | 62.14 |
| | ATOM | 1942 | CG | LEU | 549 | 16.461 | -12.191 | -0.753 | 1.00 | 60.76 |
| | ATOM | 1943 | CD1 | LEU | 549 | 17.699 | -13.074 | -0.878 | 1.00 | 57.77 |
| | ATOM | 1944 | CD2 | LEU | 549 | 15.823 | -11.972 | -2.108 | 1.00 | 58.38 |
| 25 | ATOM | 1945 | C | LEU | 549 | 13.431 | -12.574 | 1.702 | 1.00 | 66.65 |
| | ATOM | 1946 | O | LEU | 549 | 12.759 | -13.600 | 1.577 | 1.00 | 67.15 |
| | ATOM | 1947 | N | HIS | 550 | 13.541 | -11.920 | 2.856 | 1.00 | 67.72 |
| | ATOM | 1948 | CA | HIS | 550 | 12.858 | -12.378 | 4.065 | 1.00 | 69.93 |
| | ATOM | 1949 | CB | HIS | 550 | 13.753 | -12.190 | 5.298 | 1.00 | 70.76 |
| 30 | ATOM | 1950 | CG | HIS | 550 | 14.977 | -13.054 | 5.306 | 1.00 | 71.50 |
| | ATOM | 1951 | CD2 | HIS | 550 | 15.539 | -13.821 | 4.341 | 1.00 | 71.63 |
| | ATOM | 1952 | ND1 | HIS | 550 | 15.793 | -13.172 | 6.411 | 1.00 | 71.98 |
| | ATOM | 1953 | CE1 | HIS | 550 | 16.805 | -13.972 | 6.126 | 1.00 | 72.04 |
| | ATOM | 1954 | NE2 | HIS | 550 | 16.674 | -14.379 | 4.876 | 1.00 | 71.39 |
| 35 | ATOM | 1955 | C | HIS | 550 | 11.556 | -11.603 | 4.275 | 1.00 | 71.15 |
| | ATOM | 1956 | O | HIS | 550 | 10.940 | -11.684 | 5.340 | 1.00 | 70.66 |
| | ATOM | 1957 | N | ALA | 551 | 11.143 | -10.851 | 3.258 | 1.00 | 72.22 |
| | ATOM | 1958 | CA | ALA | 551 | 9.919 | -10.057 | 3.338 | 1.00 | 73.58 |
| | ATOM | 1959 | CB | ALA | 551 | 9.904 | -9.014 | 2.221 | 1.00 | 73.21 |
| 40 | ATOM | 1960 | C | ALA | 551 | 8.658 | -10.920 | 3.266 | 1.00 | 74.69 |
| | ATOM | 1961 | O | ALA | 551 | 7.684 | -10.474 | 2.621 | 1.00 | 76.12 |
| | ATOM | 1962 | OXT | ALA | 551 | 8.651 | -12.025 | 3.852 | 1.00 | 73.79 |
| | HETATM | 1963 | C10 | OHT | 600 | 30.581 | 1.481 | 29.471 | 1.00 | 26.84 |
| | HETATM | 1964 | C9 | OHT | 600 | 30.713 | -0.043 | 29.358 | 1.00 | 22.85 |
| 45 | HETATM | 1965 | C8 | OHT | 600 | 31.366 | -0.385 | 28.037 | 1.00 | 25.56 |
| | HETATM | 1966 | C11 | OHT | 600 | 32.761 | 0.051 | 27.916 | 1.00 | 27.51 |
| | HETATM | 1967 | C16 | OHT | 600 | 33.218 | 0.797 | 26.797 | 1.00 | 28.35 |
| | HETATM | 1968 | C15 | OHT | 600 | 34.551 | 1.237 | 26.747 | 1.00 | 30.39 |
| | HETATM | 1969 | C14 | OHT | 600 | 35.443 | 0.923 | 27.792 | 1.00 | 30.23 |
| 50 | HETATM | 1970 | C13 | OHT | 600 | 35.004 | 0.185 | 28.890 | 1.00 | 31.45 |
| | HETATM | 1971 | C12 | OHT | 600 | 33.666 | -0.241 | 28.955 | 1.00 | 27.93 |
| | HETATM | 1972 | C7 | OHT | 600 | 30.682 | -1.089 | 27.077 | 1.00 | 24.41 |
| | HETATM | 1973 | C1 | OHT | 600 | 29.211 | -1.258 | 27.052 | 1.00 | 24.26 |
| | HETATM | 1974 | C2 | OHT | 600 | 28.644 | -2.526 | 26.706 | 1.00 | 25.92 |
| 55 | HETATM | 1975 | C3 | OHT | 600 | 27.254 | -2.668 | 26.580 | 1.00 | 26.32 |
| | HETATM | 1976 | C4 | OHT | 600 | 26.438 | -1.553 | 26.813 | 1.00 | 29.02 |
| | HETATM | 1977 | O4 | OHT | 600 | 25.072 | -1.605 | 26.716 | 1.00 | 28.42 |
| | HETATM | 1978 | C5 | OHT | 600 | 26.980 | -0.286 | 27.130 | 1.00 | 26.98 |
| | HETATM | 1979 | C6 | OHT | 600 | 28.362 | -0.147 | 27.231 | 1.00 | 25.23 |
| 60 | HETATM | 1980 | C17 | OHT | 600 | 31.370 | -1.692 | 25.942 | 1.00 | 26.61 |
| | HETATM | 1981 | C18 | OHT | 600 | 32.508 | -2.498 | 26.151 | 1.00 | 26.77 |

| | | | | | | | | | | |
|----|--------|------|-----|-----|-----|--------|---------|--------|------|-------|
| 5 | HETATM | 1982 | C19 | OHT | 600 | 33.166 | -3.052 | 25.072 | 1.00 | 27.50 |
| | HETATM | 1983 | C20 | OHT | 600 | 32.676 | -2.794 | 23.786 | 1.00 | 27.50 |
| | HETATM | 1984 | O20 | OHT | 600 | 33.206 | -3.566 | 22.795 | 1.00 | 31.35 |
| | HETATM | 1985 | C23 | OHT | 600 | 33.009 | -3.135 | 21.448 | 1.00 | 40.09 |
| | HETATM | 1986 | C24 | OHT | 600 | 34.226 | -3.490 | 20.575 | 1.00 | 44.80 |
| 10 | HETATM | 1987 | N24 | OHT | 600 | 34.141 | -4.901 | 20.203 | 1.00 | 49.00 |
| | HETATM | 1988 | C25 | OHT | 600 | 33.375 | -5.040 | 18.933 | 1.00 | 51.64 |
| | HETATM | 1989 | C26 | OHT | 600 | 35.495 | -5.459 | 20.004 | 1.00 | 52.06 |
| | HETATM | 1990 | C21 | OHT | 600 | 31.540 | -2.005 | 23.558 | 1.00 | 27.19 |
| | HETATM | 1991 | C22 | OHT | 600 | 30.892 | -1.450 | 24.645 | 1.00 | 27.92 |
| 15 | HETATM | 1992 | O1 | HOH | 1 | 20.714 | -12.010 | 23.057 | 1.00 | 27.20 |
| | HETATM | 1993 | O1 | HOH | 2 | 22.563 | -0.070 | 25.819 | 1.00 | 25.77 |
| | HETATM | 1994 | O1 | HOH | 3 | 25.183 | 19.202 | 23.149 | 1.00 | 42.52 |
| | HETATM | 1995 | O1 | HOH | 4 | 35.158 | 5.823 | 37.390 | 1.00 | 33.92 |
| | HETATM | 1996 | O1 | HOH | 5 | 22.116 | -9.922 | 18.914 | 1.00 | 30.18 |
| 20 | HETATM | 1997 | O1 | HOH | 6 | 29.812 | 6.536 | 19.652 | 1.00 | 26.11 |
| | HETATM | 1998 | O1 | HOH | 7 | 13.362 | 4.463 | 20.376 | 1.00 | 29.40 |
| | HETATM | 1999 | O1 | HOH | 8 | 19.799 | -11.295 | 20.187 | 1.00 | 28.70 |
| | HETATM | 2000 | O1 | HOH | 9 | 21.205 | 1.466 | 23.794 | 1.00 | 22.47 |
| | HETATM | 2001 | O1 | HOH | 10 | 21.177 | -4.961 | 29.066 | 1.00 | 33.00 |
| 25 | HETATM | 2002 | O1 | HOH | 11 | 18.591 | 1.863 | 20.518 | 1.00 | 32.59 |
| | HETATM | 2003 | O1 | HOH | 12 | 16.298 | 21.566 | 15.992 | 1.00 | 33.42 |
| | HETATM | 2004 | O1 | HOH | 13 | 18.611 | 1.976 | 24.494 | 1.00 | 29.70 |
| | HETATM | 2005 | O1 | HOH | 14 | 38.009 | 8.910 | 21.156 | 1.00 | 39.92 |
| | HETATM | 2006 | O1 | HOH | 15 | 26.549 | 11.664 | 18.080 | 1.00 | 30.25 |
| 30 | HETATM | 2007 | O1 | HOH | 16 | 20.282 | -4.239 | 26.512 | 1.00 | 32.70 |
| | HETATM | 2008 | O1 | HOH | 17 | 32.858 | 8.754 | 20.237 | 1.00 | 29.88 |
| | HETATM | 2009 | O1 | HOH | 18 | 8.497 | 16.136 | 29.934 | 1.00 | 46.80 |
| | HETATM | 2010 | O1 | HOH | 19 | 21.940 | 19.301 | 31.632 | 1.00 | 35.72 |
| | HETATM | 2011 | O1 | HOH | 20 | 35.153 | 2.682 | 14.122 | 1.00 | 41.02 |
| 35 | HETATM | 2012 | O1 | HOH | 21 | 20.358 | -2.268 | 21.013 | 1.00 | 29.43 |
| | HETATM | 2013 | O1 | HOH | 22 | 35.562 | 10.036 | 36.334 | 1.00 | 41.37 |
| | HETATM | 2014 | O1 | HOH | 23 | 17.248 | 18.187 | 17.571 | 1.00 | 33.96 |
| | HETATM | 2015 | O1 | HOH | 24 | 18.445 | 20.973 | 12.346 | 1.00 | 43.44 |
| | HETATM | 2016 | O1 | HOH | 25 | 12.152 | 23.054 | 33.132 | 1.00 | 36.04 |
| 40 | HETATM | 2017 | O1 | HOH | 26 | 13.181 | 22.222 | 9.699 | 1.00 | 37.03 |
| | HETATM | 2018 | O1 | HOH | 27 | 19.399 | -6.090 | 12.808 | 1.00 | 44.86 |
| | HETATM | 2019 | O1 | HOH | 28 | 37.895 | 13.599 | 31.395 | 1.00 | 47.26 |
| | HETATM | 2020 | O1 | HOH | 29 | 11.570 | 6.212 | 7.962 | 1.00 | 51.10 |
| | HETATM | 2021 | O1 | HOH | 30 | 20.172 | -2.568 | 23.445 | 1.00 | 51.70 |
| 45 | HETATM | 2022 | O1 | HOH | 31 | 36.402 | -5.369 | 23.729 | 1.00 | 58.20 |
| | HETATM | 2023 | O1 | HOH | 32 | 25.127 | 13.802 | 19.187 | 1.00 | 35.29 |
| | HETATM | 2024 | O1 | HOH | 33 | 23.181 | 4.937 | 38.538 | 1.00 | 33.77 |
| | HETATM | 2025 | O1 | HOH | 34 | 20.550 | 0.421 | 21.276 | 1.00 | 29.12 |
| | HETATM | 2026 | O1 | HOH | 35 | 39.599 | 13.954 | 27.312 | 1.00 | 44.08 |
| 50 | HETATM | 2027 | O1 | HOH | 36 | 26.445 | 13.863 | 21.285 | 1.00 | 34.97 |
| | HETATM | 2028 | O1 | HOH | 37 | 13.759 | 5.079 | 9.108 | 1.00 | 38.54 |
| | HETATM | 2029 | O1 | HOH | 38 | 14.150 | 24.731 | 34.529 | 1.00 | 49.72 |
| | HETATM | 2030 | O1 | HOH | 39 | 21.060 | 13.886 | -6.319 | 1.00 | 59.79 |
| | HETATM | 2031 | O1 | HOH | 40 | 32.215 | 6.217 | 8.726 | 1.00 | 60.22 |
| 55 | HETATM | 2032 | O1 | HOH | 41 | 35.105 | 15.704 | 9.069 | 1.00 | 45.15 |
| | HETATM | 2033 | O1 | HOH | 42 | 11.427 | 19.451 | 9.903 | 1.00 | 38.56 |
| | HETATM | 2034 | O1 | HOH | 43 | 19.662 | 23.472 | 10.333 | 1.00 | 47.71 |
| | HETATM | 2035 | O1 | HOH | 44 | 9.231 | 3.690 | 12.337 | 1.00 | 45.98 |
| | HETATM | 2036 | O1 | HOH | 45 | 15.313 | -6.036 | 17.192 | 1.00 | 39.07 |
| 60 | HETATM | 2037 | O1 | HOH | 46 | 15.517 | -3.266 | 17.907 | 1.00 | 37.67 |
| | HETATM | 2038 | O1 | HOH | 47 | 28.784 | -16.713 | 25.163 | 1.00 | 55.44 |

| | | | | | | | | | | |
|----|--------|------|----|-----|----|--------|---------|--------|------|-------|
| 5 | HETATM | 2039 | O1 | HOH | 48 | 27.868 | -10.898 | 28.271 | 1.00 | 31.27 |
| | HETATM | 2040 | O1 | HOH | 49 | 6.955 | 13.568 | 28.233 | 1.00 | 48.83 |
| | HETATM | 2041 | O1 | HOH | 50 | 22.051 | -15.030 | 28.603 | 1.00 | 36.91 |
| | HETATM | 2042 | O1 | HOH | 51 | 7.026 | 31.002 | 30.284 | 1.00 | 46.73 |
| | HETATM | 2043 | O1 | HOH | 52 | -1.489 | 12.385 | 15.164 | 1.00 | 51.17 |
| 10 | HETATM | 2044 | O1 | HOH | 53 | 3.499 | 6.444 | 14.452 | 1.00 | 50.38 |
| | HETATM | 2045 | O1 | HOH | 54 | 18.655 | -2.048 | 25.518 | 1.00 | 52.29 |
| | HETATM | 2046 | O1 | HOH | 55 | 28.188 | -15.195 | 38.996 | 1.00 | 55.22 |
| | HETATM | 2047 | O1 | HOH | 56 | 35.275 | -10.556 | 38.061 | 1.00 | 57.39 |
| | HETATM | 2048 | O1 | HOH | 57 | 37.771 | -9.103 | 34.605 | 1.00 | 54.17 |
| 15 | HETATM | 2049 | O1 | HOH | 58 | 31.403 | -3.039 | 17.983 | 1.00 | 46.80 |
| | HETATM | 2050 | O1 | HOH | 59 | 30.455 | -6.352 | 17.005 | 1.00 | 47.05 |
| | HETATM | 2051 | O1 | HOH | 60 | 25.985 | 8.255 | 0.416 | 1.00 | 43.32 |
| | HETATM | 2052 | O1 | HOH | 61 | 35.679 | 0.749 | 10.462 | 1.00 | 42.99 |
| | HETATM | 2053 | O1 | HOH | 62 | 14.741 | 4.029 | 33.936 | 1.00 | 49.59 |
| 20 | HETATM | 2054 | O1 | HOH | 63 | 16.333 | 2.592 | 35.952 | 1.00 | 45.13 |
| | HETATM | 2055 | O1 | HOH | 64 | 23.809 | 7.186 | 39.798 | 1.00 | 45.36 |
| | HETATM | 2056 | O1 | HOH | 65 | 27.012 | -1.948 | 46.995 | 1.00 | 63.39 |
| | HETATM | 2057 | O1 | HOH | 66 | 25.956 | -6.422 | 42.144 | 1.00 | 44.94 |
| | HETATM | 2058 | O1 | HOH | 67 | 23.510 | -8.414 | 39.036 | 1.00 | 39.06 |
| 25 | HETATM | 2059 | O1 | HOH | 68 | 41.475 | 0.971 | 33.110 | 1.00 | 55.50 |
| | HETATM | 2060 | O1 | HOH | 69 | 36.519 | 8.863 | 38.836 | 1.00 | 41.56 |
| | HETATM | 2061 | O1 | HOH | 70 | 30.111 | 14.823 | 12.793 | 1.00 | 44.58 |
| | HETATM | 2062 | O1 | HOH | 71 | 26.850 | -6.092 | 1.594 | 1.00 | 40.15 |
| | HETATM | 2063 | O1 | HOH | 72 | 20.448 | -3.169 | 1.055 | 1.00 | 42.50 |
| 30 | HETATM | 2064 | O1 | HOH | 73 | 33.896 | 3.047 | 16.172 | 1.00 | 46.39 |
| | HETATM | 2065 | O1 | HOH | 74 | 16.884 | 0.446 | 26.043 | 1.00 | 61.50 |
| | HETATM | 2066 | O1 | HOH | 75 | 18.595 | 0.296 | 27.866 | 1.00 | 47.33 |
| | HETATM | 2067 | O1 | HOH | 76 | 6.166 | 21.439 | 19.124 | 1.00 | 47.94 |
| | HETATM | 2068 | O1 | HOH | 77 | 18.484 | 20.060 | 16.232 | 1.00 | 35.52 |
| 35 | HETATM | 2069 | O1 | HOH | 78 | 1.985 | 23.265 | 29.187 | 1.00 | 46.42 |
| | HETATM | 2070 | O1 | HOH | 79 | 12.729 | 30.461 | 27.530 | 1.00 | 62.79 |
| | END | | | | | | | | | |

5 WHAT IS CLAIMED IS:

1. A method of identifying a compound that modulates coactivator binding to a nuclear receptor, said method comprising:

10 modeling test compounds that fit spacially into a nuclear receptor coactivator binding site of interest using an atomic structural model of a nuclear receptor coactivator binding site or portion thereof,

screening said test compounds in an assay characterized by binding of a test compound to a nuclear receptor coactivator binding site, and

15 identifying a test compound that modulates coactivator binding to said nuclear receptor.

2. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of Val284, Phe293, Ile302, Leu305, and Leu454.

20

3. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of Val284, Lys288, Ile302, Lys306, Leu454 and Glu457.

25

4. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.

30

5. The method of claim 1, wherein said nuclear receptor coactivator binding site comprises amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and
35 helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.

6. The method of claim 5, wherein said amino acid residues corresponding to residues of human thyroid receptor comprise Val284, Phe293, Ile302, Leu305, and Leu454.

7. The method of claim 5, wherein said amino acid residues corresponding to residues of human thyroid receptor comprise Val284, Lys288, Ile302, Lys306, Leu454 and Glu457.

8. The method of claim 1, wherein said nuclear receptor coactivator binding site
10 comprises amino acid residues corresponding to residues of human thyroid receptor of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.

15 9. The method of any one of claims 5 through 8, wherein said nuclear receptor is selected from the group consisting of TR, RAR, RXR, PPAR, VDR, ER, GR, PR, MR, and AR.

10. The method of claim 1, wherein said screening is *in vitro*.

20 11. The method of claim 10, wherein said screening is high throughput screening.

12. The method of claim 1, wherein said assay is a biological assay.

13. The method of claim 1, wherein said test compound is from a library of compounds.
25

14. The method of claim 1, wherein said test compound is an agonist or antagonist of coactivator binding.

15. The method of claim 14, wherein said test compound is a small organic molecule, a
30 peptide, or peptidomimetic.

16. The method of claim 15, wherein said compound is a peptide comprising a NR-box amino acid sequence, or derivative thereof.

35 17. A method for identifying an agonist or antagonist of coactivator binding to a nuclear receptor, said method comprising the steps of:

providing the atomic coordinates of a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system;

5 modeling compounds which fit spacially into the nuclear receptor coactivator binding site; and

identifying in an assay for nuclear receptor activity a compound that increases or decreases the activity of said nuclear receptor by binding the coactivator binding site of said nuclear receptor, whereby an agonist or antagonist of coactivator binding is identified.

10

18. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecular complex of a compound bound to a nuclear receptor coactivator binding site comprising
15 structure coordinates of amino acids corresponding to human thyroid receptor amino acids selected from the group consisting of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459, or a homologue of said molecular complex, wherein said homologue comprises a coactivator binding site that has a root
20 mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

19. The machine readable storage medium of claim 18, wherein said nuclear receptor is a thyroid receptor.

25 20. The machine readable storage medium of claim 19, wherein said thyroid receptor is human.

21. The machine readable storage medium of claim 20, wherein said molecule is peptide

30 22. The machine readable storage medium of claim 21, wherein said peptide comprises a NR-box amino acid sequence, or derivative thereof.

23. The machine-readable data storage medium according to claim 18, wherein said molecular complex is defined by the set of structure coordinates depicted in Appendix 1, or a
35 homologue of said molecular complex, said homologue having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

- 5 24. A machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data which, when combined with a second set of machine readable data, using a machine programmed with instructions for using said first set of data and said second set of data, can determine at least a portion of the structure coordinates corresponding to the second set of machine readable data, wherein: said first set of data comprises a Fourier transform of at least a portion of the structural coordinates selected from the group consisting of coordinates depicted in Appendix 1; and said second set of data comprises an X-ray diffraction pattern of a molecule or molecular complex.
- 10

25. A cocrystal of a nuclear receptor comprising a molecule bound to the coactivator binding site of said nuclear receptor.
- 15

26. The cocrystal of claim 25, wherein said nuclear receptor is a thyroid receptor.

27. The cocrystal of claim 26, wherein said thyroid receptor is human.
- 20

28. The cocrystal of claim 27, wherein said molecule is peptide.

29. The cocrystal of claim 28, wherein said peptide comprises a NR-box amino acid sequence or derivative thereof.
- 25

30. A compound identified according to the method of claim 1.

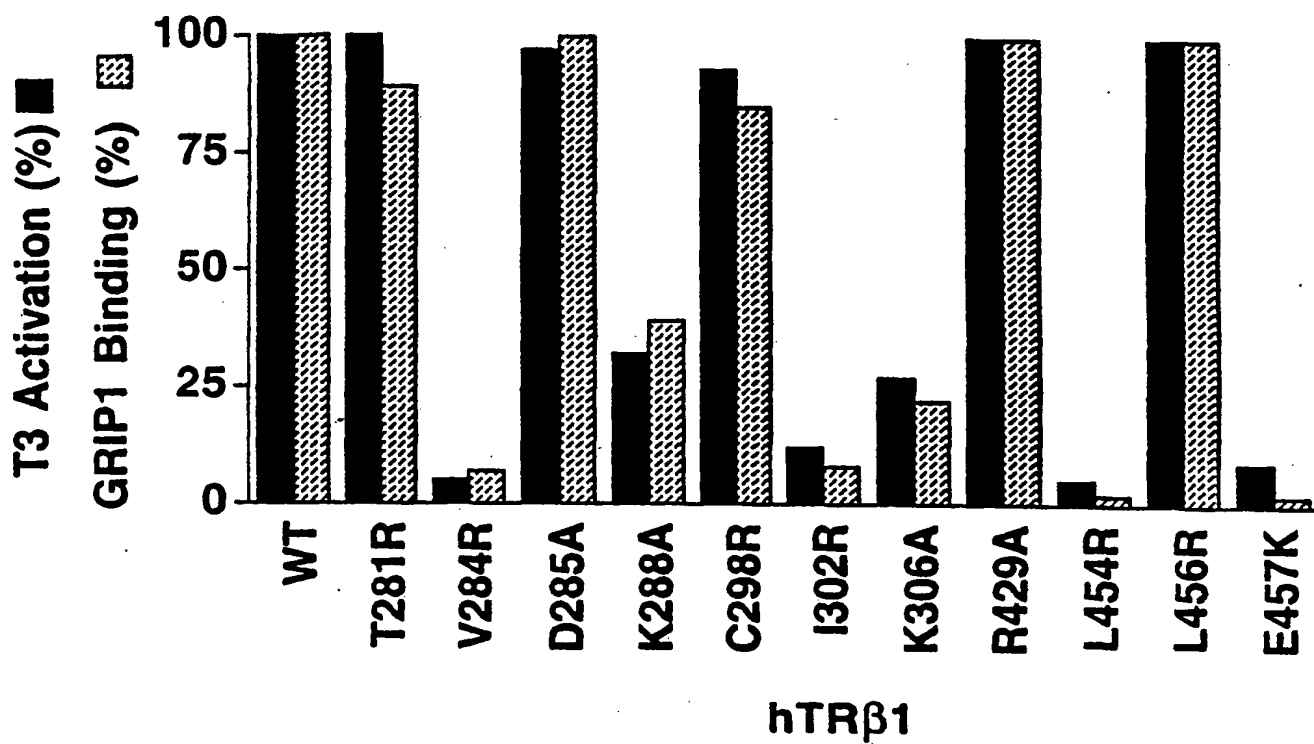
FIGURE 1

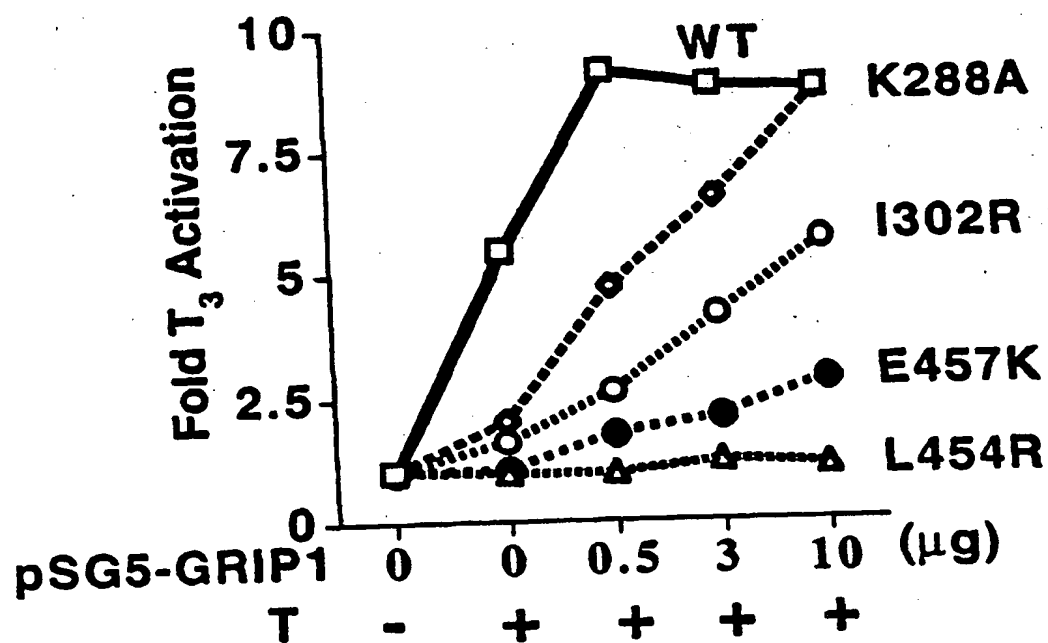
FIGURE 2

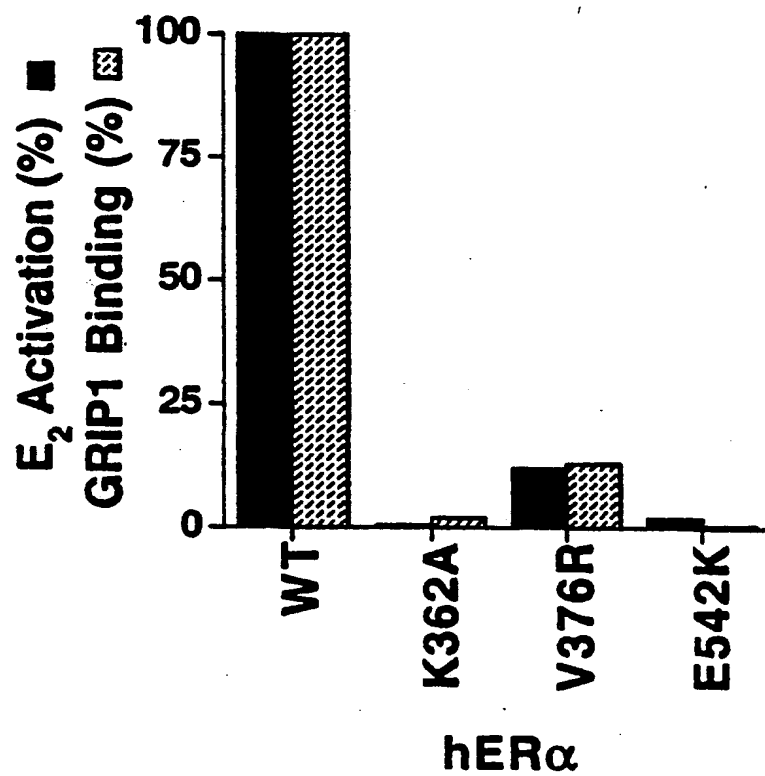
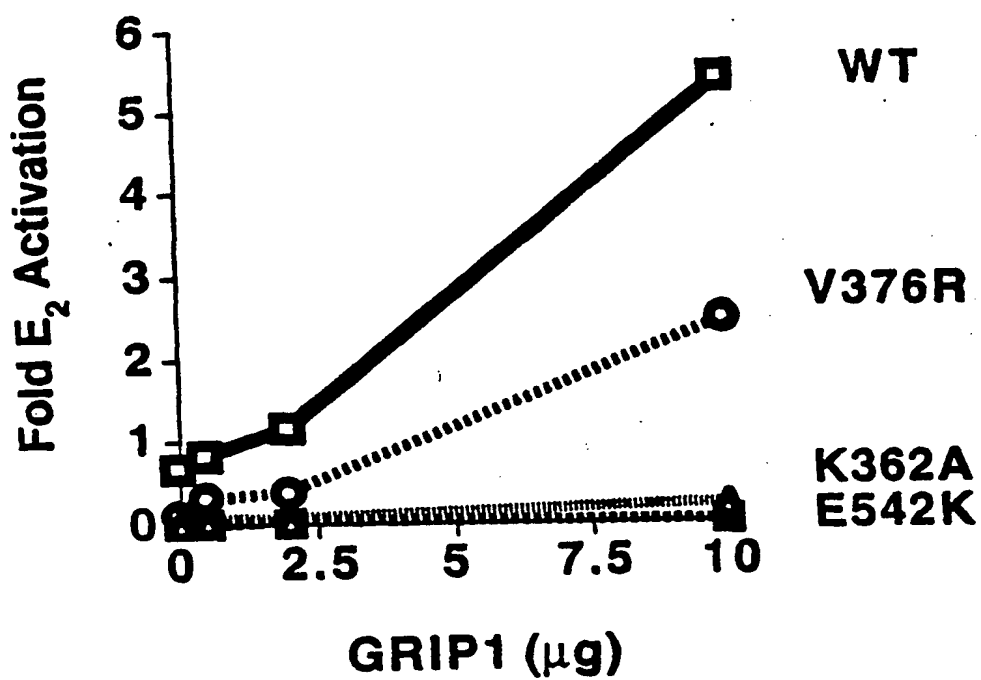
FIGURE 3

FIGURE 4

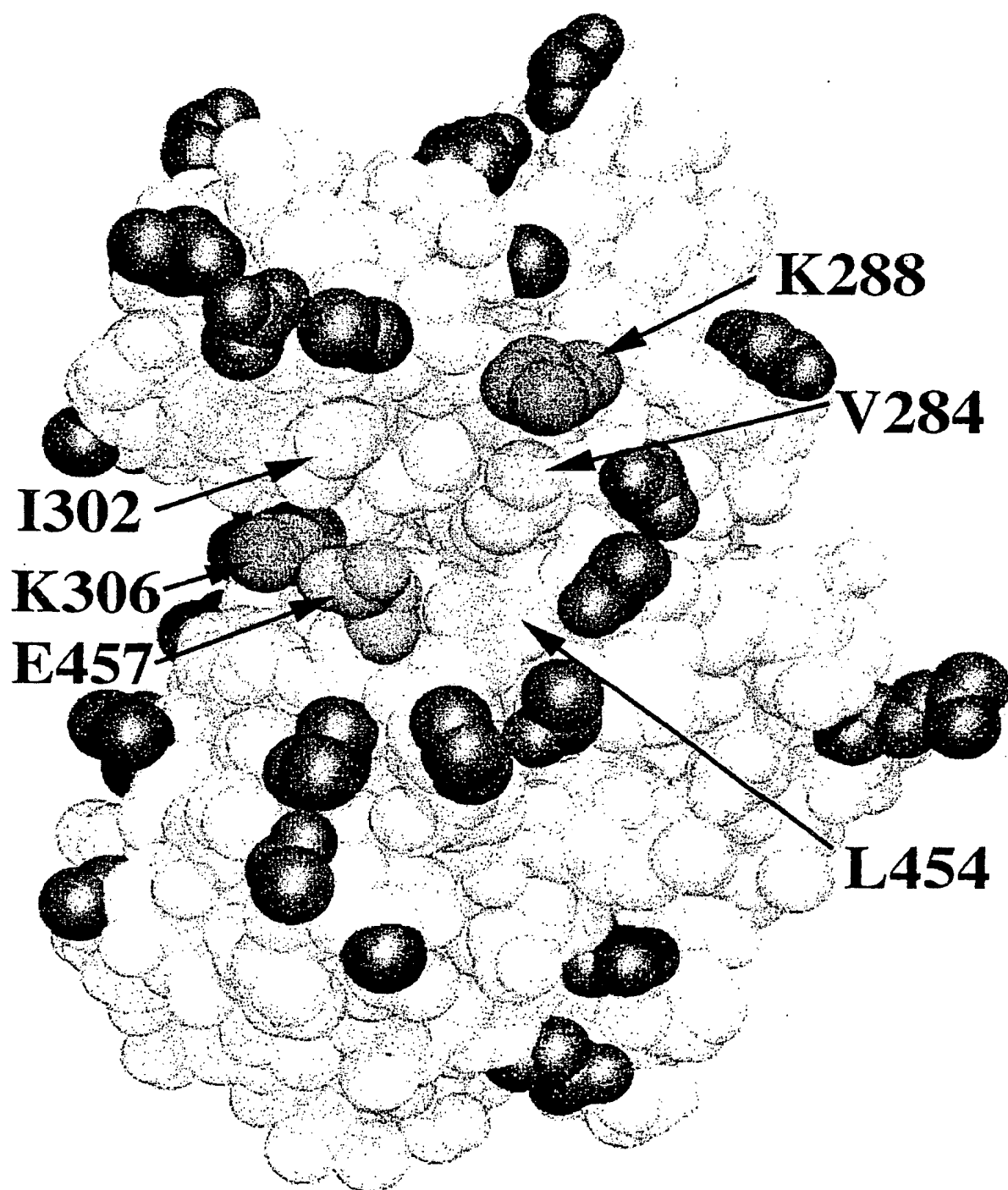
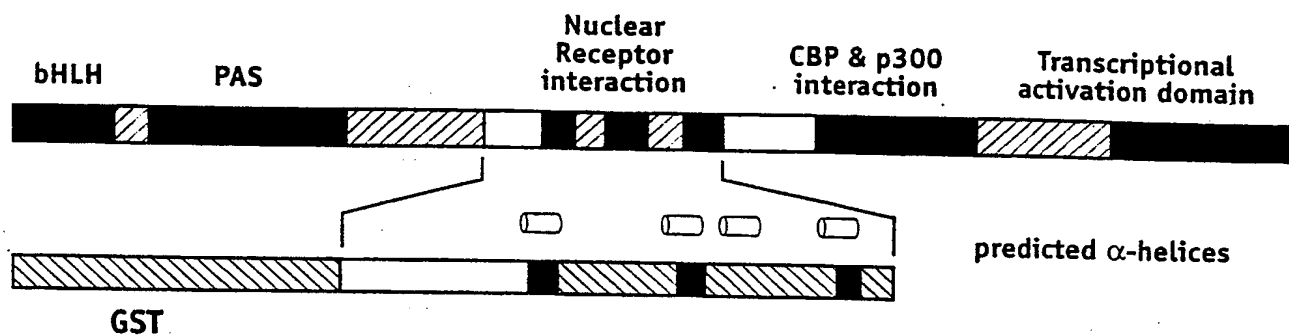
**FIG. 5**

FIGURE 6

| | bHLH | PAS | Nuclear Receptor interaction | CBP & p300 interaction | Transcriptional activation domain |
|---|------|-----|------------------------------------|-------------------------------------|--------------------------------------|
| | | | | | |
| | | | 1 | 2 | 3 |
| 1 | | | SEQ ID NO: 5 Grip1 | AEGHSRLHDSKGQTKLLQLLTTKSEQMEPSPLAS | |
| | | | SEQ ID NO: 8 Tif2 | ADGQSRLHDSKGQTKLLQLLTTKSEQMEPSPLAS | |
| | | | SEQ ID NO: 11 NcoA-2 | AEGHSRLHDSKGQTKLLQLLTTKSEQMEPSPLPS | |
| | | | SEQ ID NO: 14 RAC3 | AENQRGPLESKGHKLLQLLTCSSDDRGHSSLTN | |
| | | | SEQ ID NO: 17 AIB1, TRAM-1 | AENQRGPLESKGHKLLQLLTCSSDDRGHSSLTN | |
| | | | SEQ ID NO: 20 p/CIP | SETPRGPLESKGHKLLQLLTCSSDDRGHSSLTN | |
| | | | SEQ ID NO: 23 SRC1 | SEGDSKY--SQTSHKLVQLLTTTAEQQLRHADID | |
| | | | SEQ ID NO: 26 Consensus |S....KLhQLLT,.... | |
| 2 | | | SEQ ID NO: 6 Grip1 | PGSTHGTSLKEKHKILHRLLQDSSSPVDLAKLTA | |
| | | | SEQ ID NO: 9 Tif2 | SGSTHGTSLKEKHKILHRLLQDSSSPVDLAKLTA | |
| | | | SEQ ID NO: 12 NcoA-2 | PGSTHGTSLKEKHKILHRLLQDSSSPVDLAKLTA | |
| | | | SEQ ID NO: 15 RAC3 | TSNMHGSLLOEKHRILHKLLQNGNSPAEVAKITA | |
| | | | SEQ ID NO: 18 AIB1, TRAM-1 | TSNMHGSLLOEKHRILHKLLQNGNSPAEVAKITA | |
| | | | SEQ ID NO: 21 p/CIP | TSNVHGSLLOEKHRILHKLLQNGNSPAEVAKITA | |
| | | | SEQ ID NO: 24 SRC1 | TCPSSHSSSLTERHKILHRLLQE.GSPSDITTLVS | |
| | | | SEQ ID NO: 27 Consensus |L.E+H+ILH+LLQ...SP.-h..h.. | |
| 3 | | | SEQ ID NO: 7 Grip1 | EPASPKKKE---NALLRYLLDKDDTKDIGLPEIT | |
| | | | SEQ ID NO: 10 Tif2 | EPVSPKKKE---NALLRYLLDKDDTKDIGLPEIT | |
| | | | SEQ ID NO: 13 NcoA-2 | EPASPKKKE---NALLRYLLDKDDTKDIGLPSIT | |
| | | | SEQ ID NO: 16 RAC3 | EQLSPKKKE--NNALLRYLLDRDDPSDVLAKKLQ | |
| | | | SEQ ID NO: 19 AIB1, TRAM-1 | EQLSPKKKE--NNALLRYLLDRDDPSDALSKEIQ | |
| | | | SEQ ID NO: 22 p/CIP | EQLSPKKKE--NNALLRYLLDRDDPSDALSKEIQ | |
| | | | SEQ ID NO: 25 SRC1 | ELDAAKKKESKDHQLLYLLDKDEKDLRSTPNLC | |
| | | | SEQ ID NO: 28 Consensus | E....KKKE....LLRYLLD+D-.....h. | |
| | | | Overall Consensus (SEQ ID NO: 1) |LXXLL..... | |

FIGURE 7a



| | NR-box1 residues 15-21 SEQ ID NO: 5 | NR-box1 residues 15-21 SEQ ID NO: 6 | NR box3 residues 15-21 SEQ ID NO: 7 |
|-----------|---|---|---|
| NRb 1,2,3 | KLLQLLT | ILHRLQ | LLRYLLD |
| NRb 1,2 | KLLQLLT | ILHRLQ | AARAAAD |
| NRb 1,3 | KLLQLLT | AAHRAAQ | LLRYLLD |
| NRb 1 | KLLQLLT | AAHRAAQ | AARAAAD |

FIGURE 7b

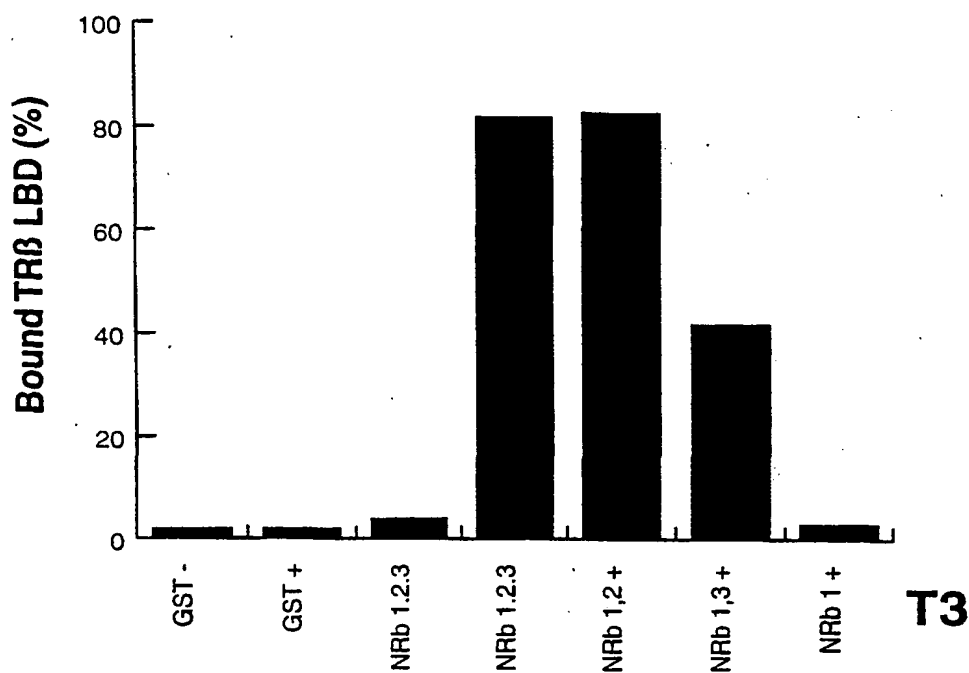


FIGURE 8a

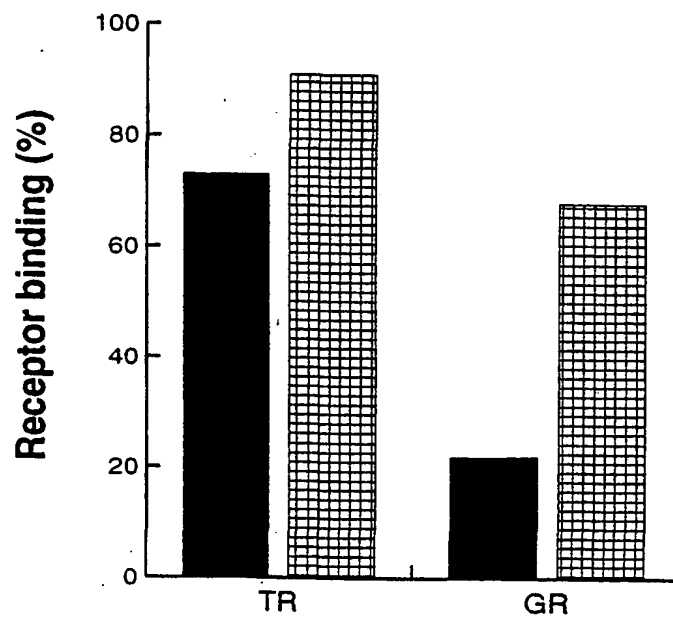
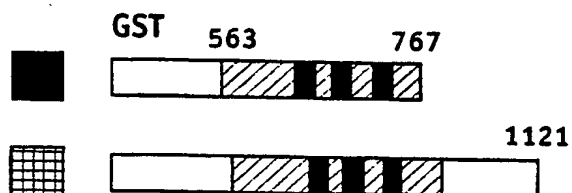


FIGURE 8b

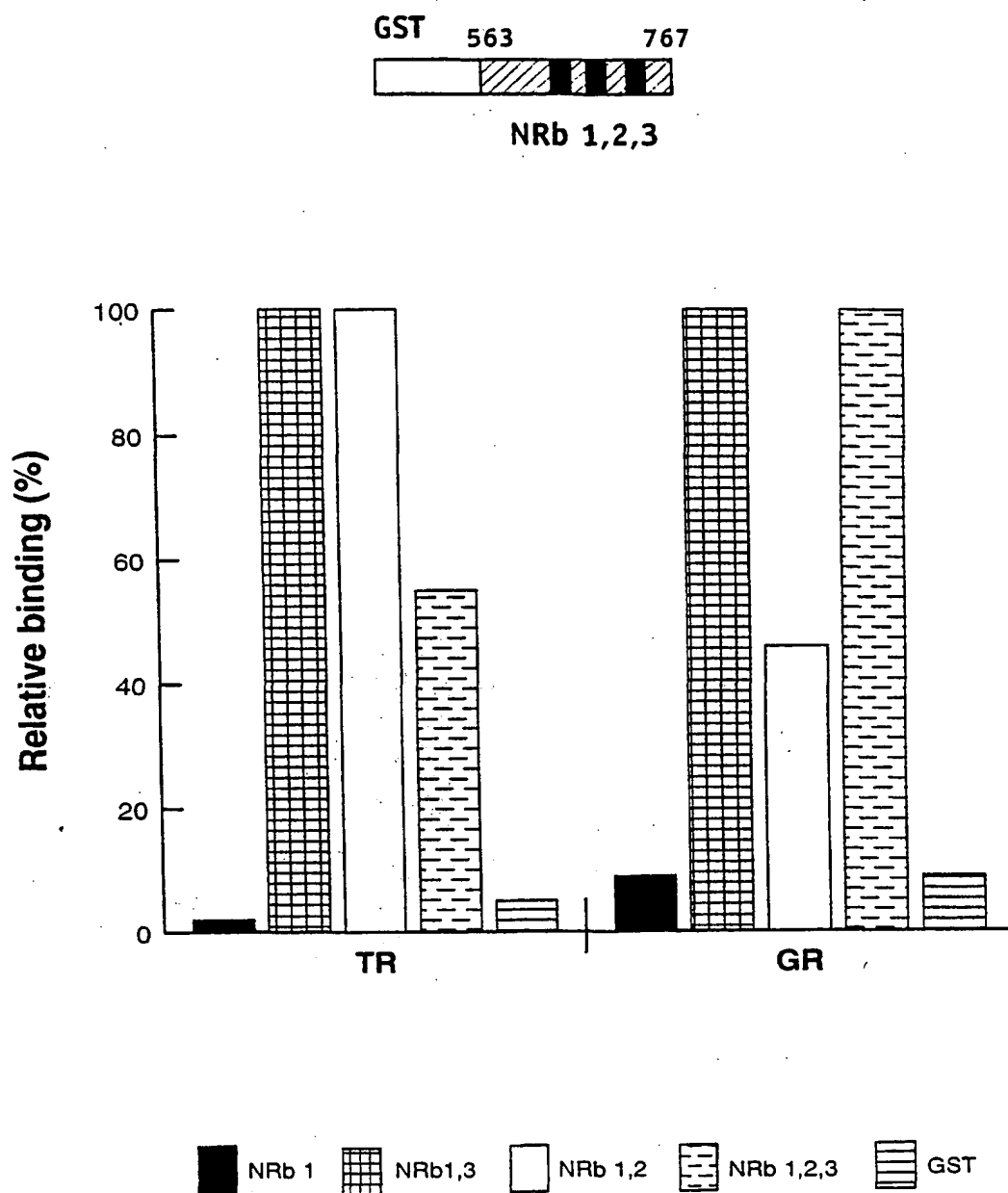


FIGURE 9a

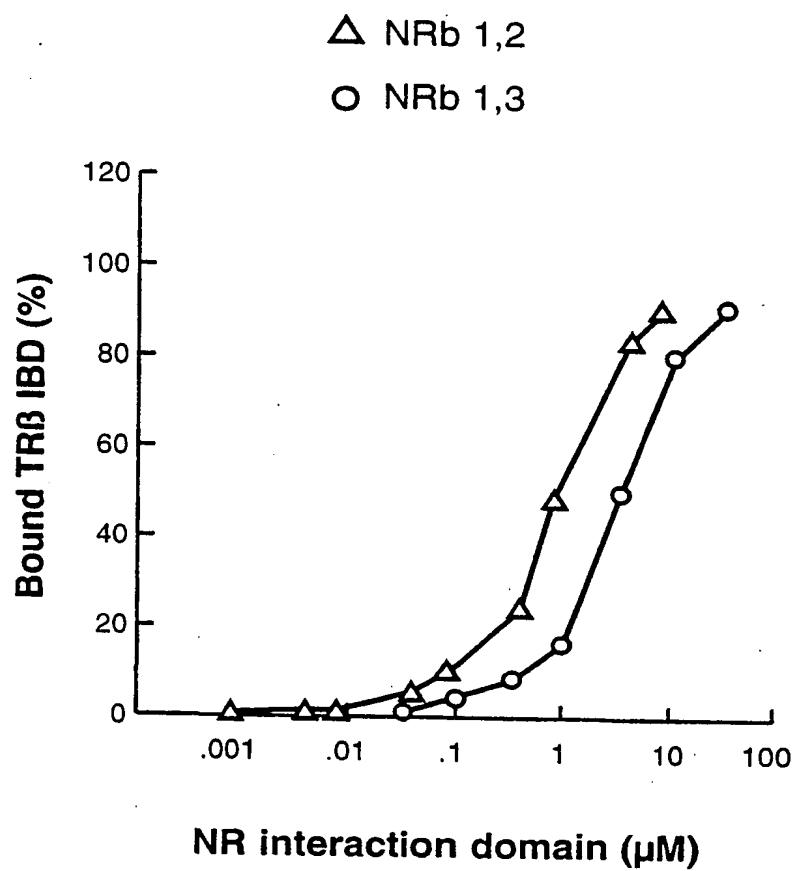
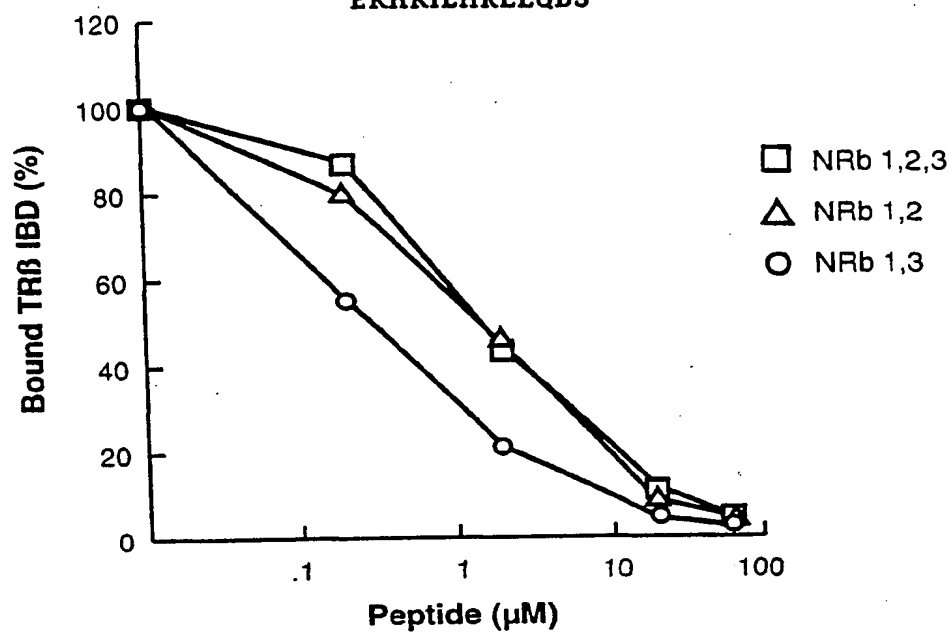
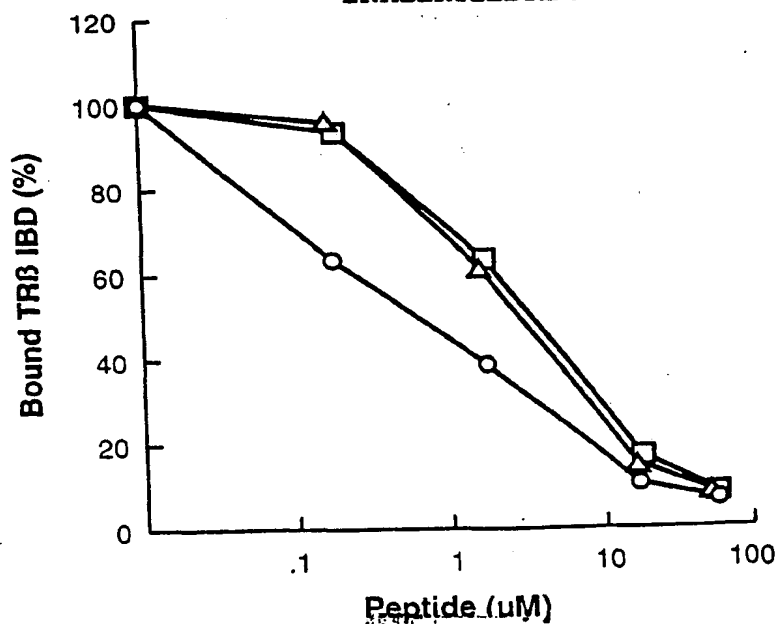


FIGURE 9b

NR-box 2 peptide
EKHKILHRLLODS



NR-box 3 peptide
ENALLRYLLDKDO



SUBSTITUTE SHEET (RULE 26)

FIGURE 10a

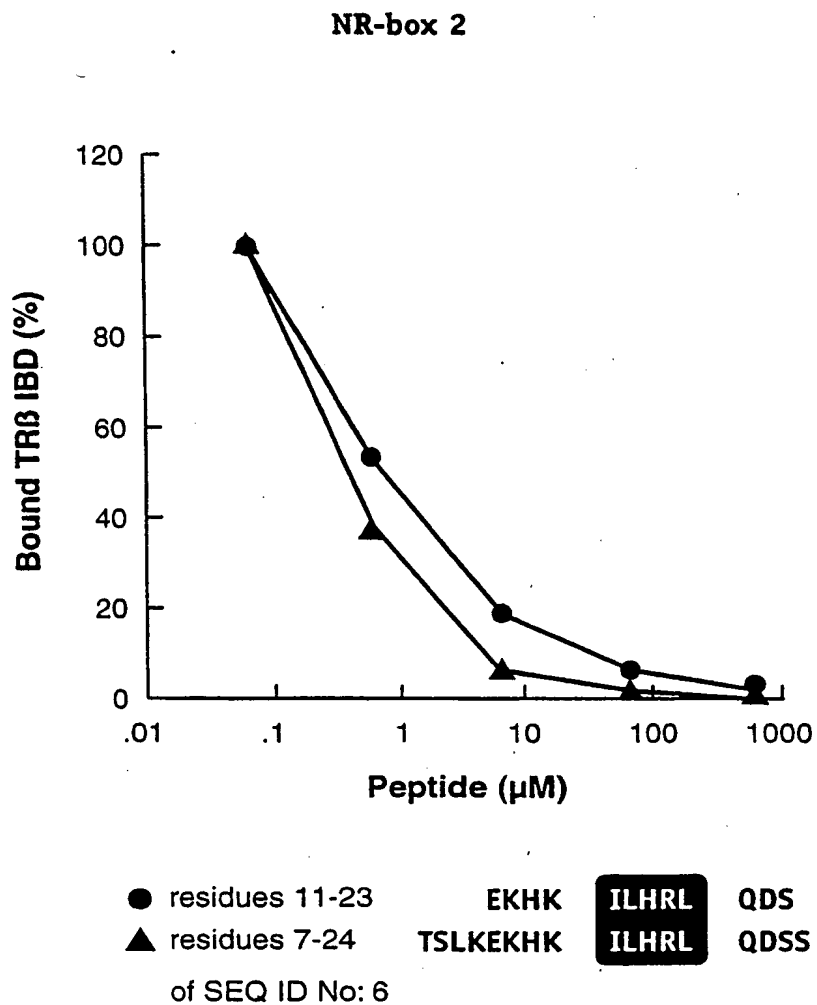


FIGURE 10b

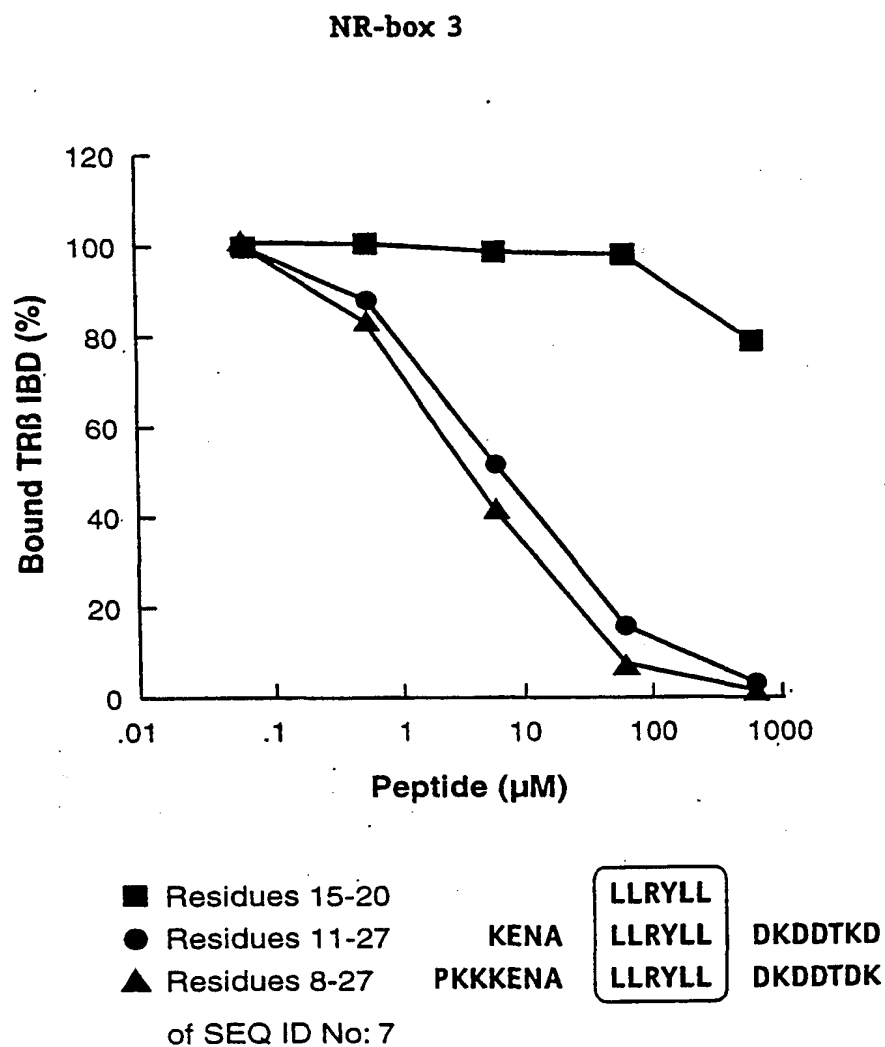
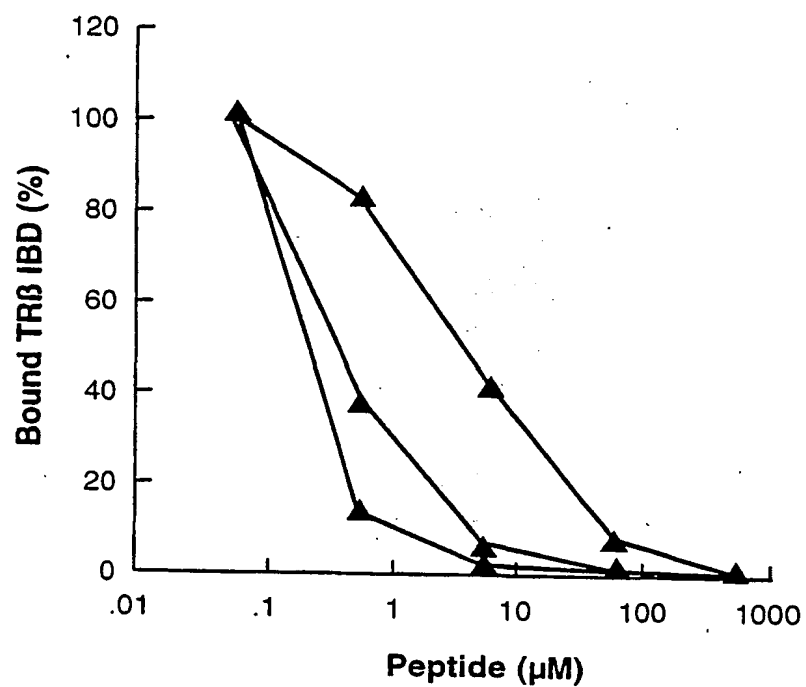
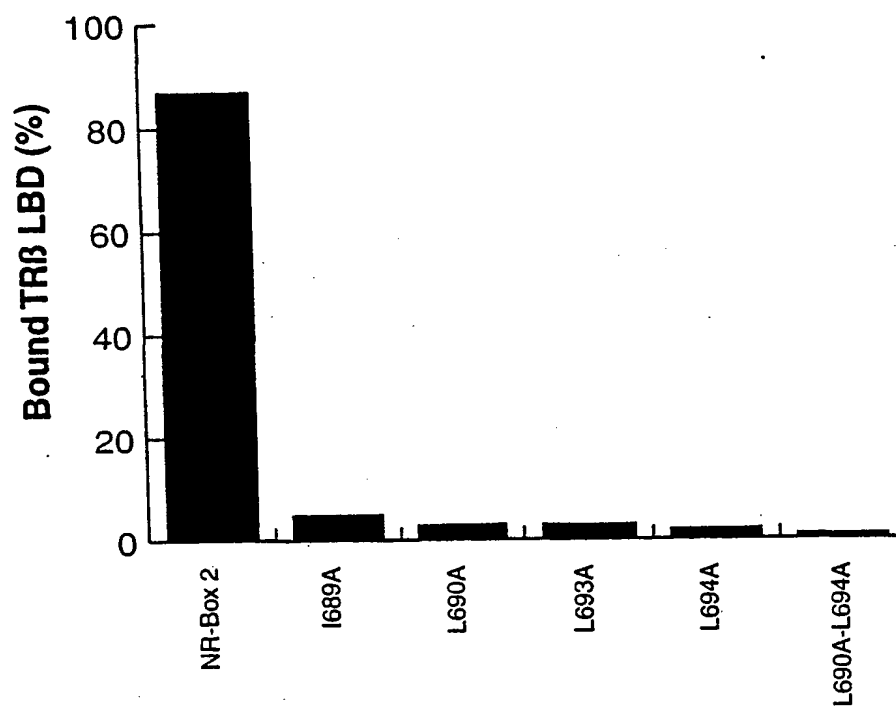


FIGURE 10c



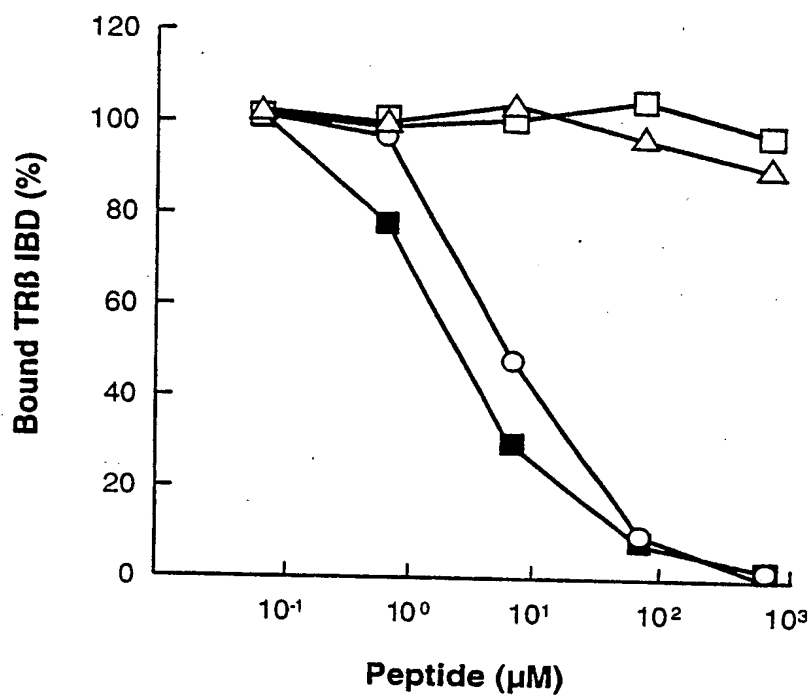
| | | | |
|----------------------------------|----------|--------|---------|
| ▲ Residues 8027 of SEQ ID No: 7 | PKKKENA | LLRYLL | DKDDTKD |
| ▲ Residues 11-27 of SEQ ID No: 6 | TSLKEKHK | LLHRLL | QDSS |
| ▲ SEQ ID No: 29 | TSLKEKHK | LLRYLL | QDSS |

FIGURE 11a



NR-interaction domain:

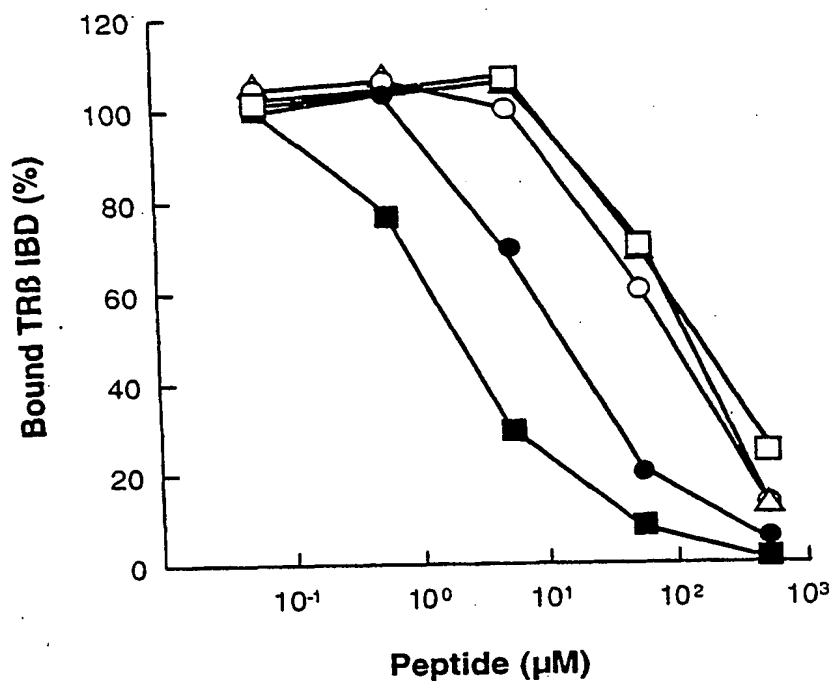
| | |
|-------------|--------|
| NRb 1,2 | ILHRLL |
| I689A | ALHRLL |
| L690A | IAHRLL |
| L693A | ILHRAL |
| L694A | ILHRLA |
| L690A/L694A | IAHRLA |

FIGURE 11b

Residues 12-24 SEQ ID No: 6

NR-Box 2 peptide: KHK **ILLHRLL** QDSS

- ILHRLL
□ AAHRLL
○ ILAALL
△ ILHRAA

FIGURE 11c

Residues 12-24 SEQ ID No: 6

NR-Box 2 peptide: KHK **ILLHRLL** QDSS

- ILHRLL
- FLHRLL
- IFHRLL
- ILHRFL
- △ ILHRLF

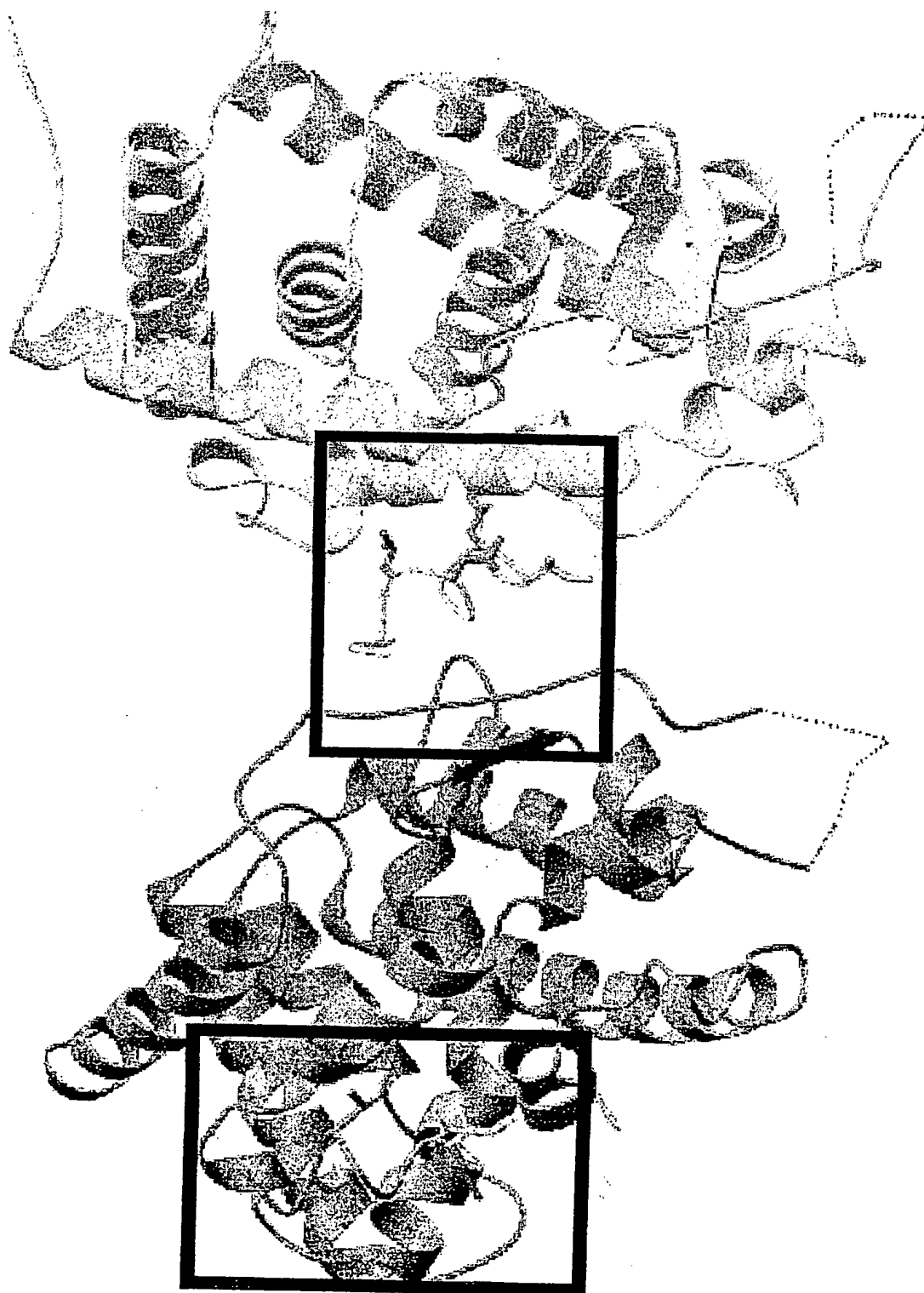


FIG. 12

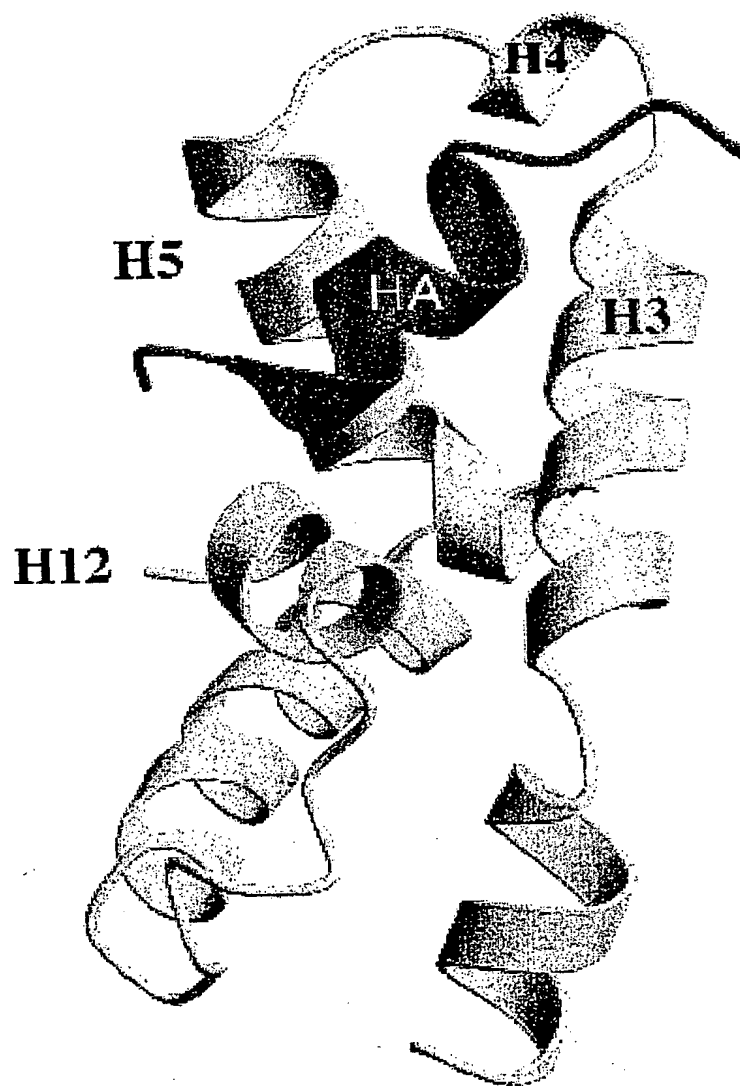
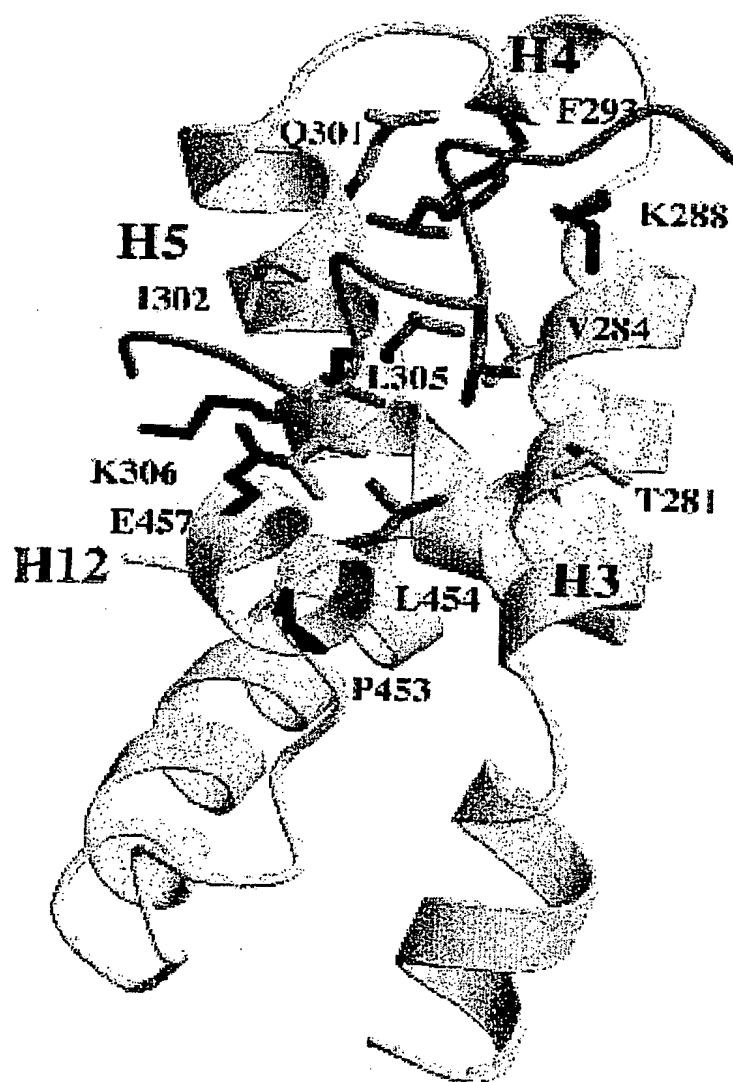
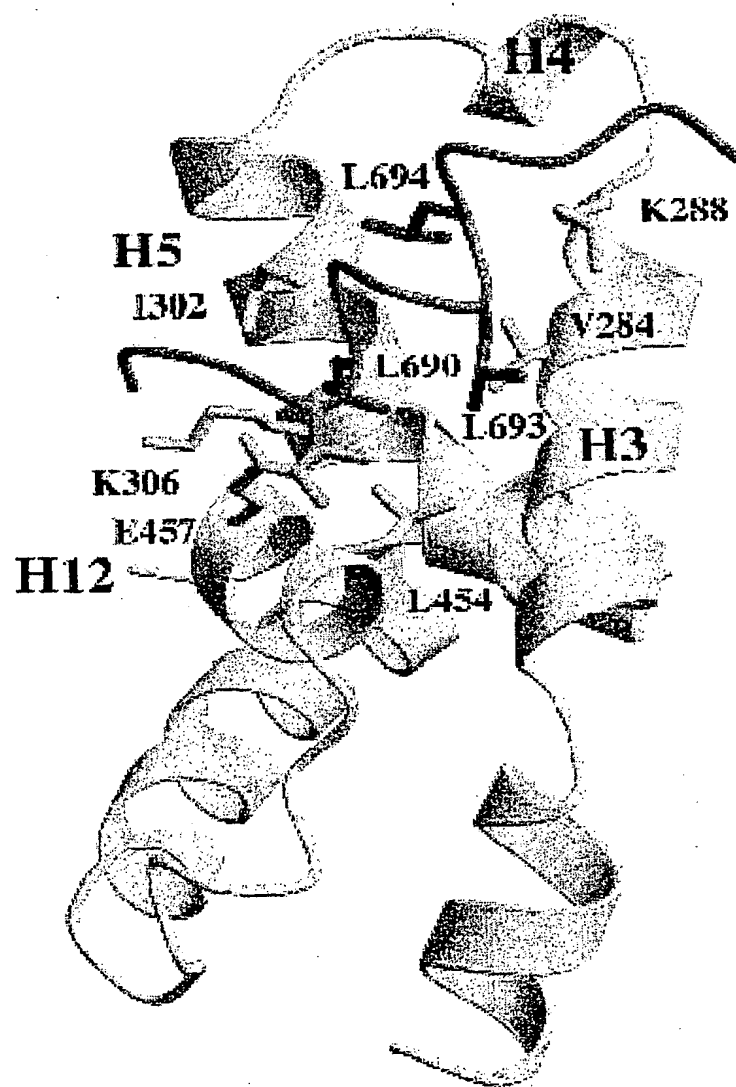


FIG. 13

**FIG. 14**

**FIG. 15**

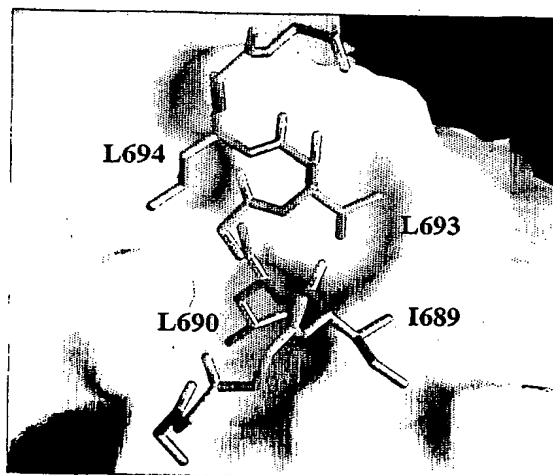


FIG. 16

SUBSTITUTE SHEET (RULE 26)

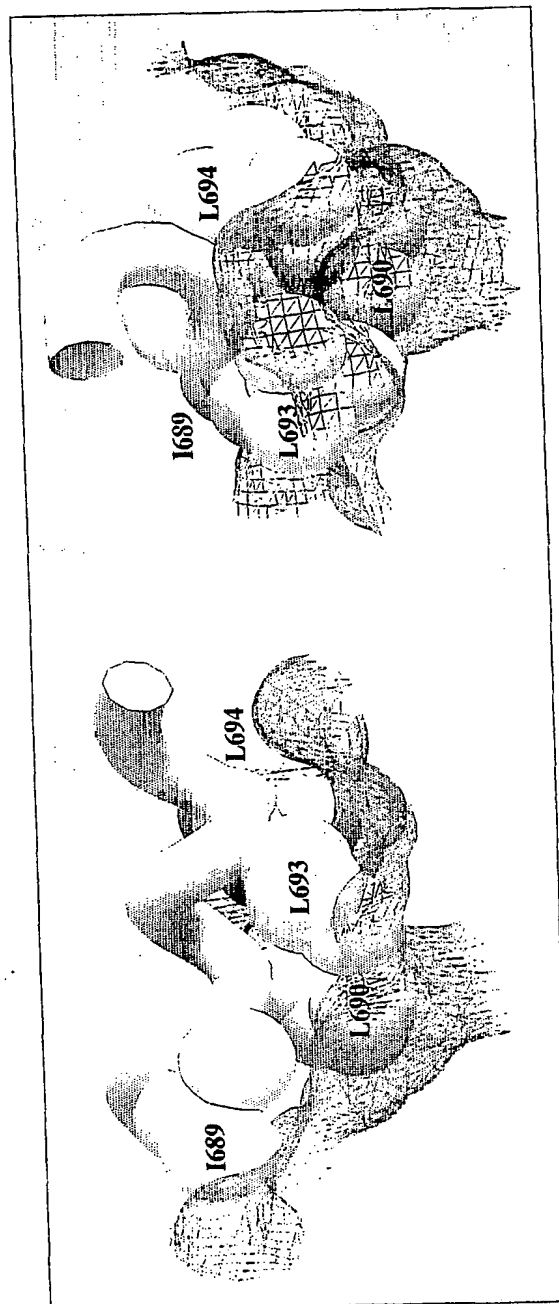


FIG. 17

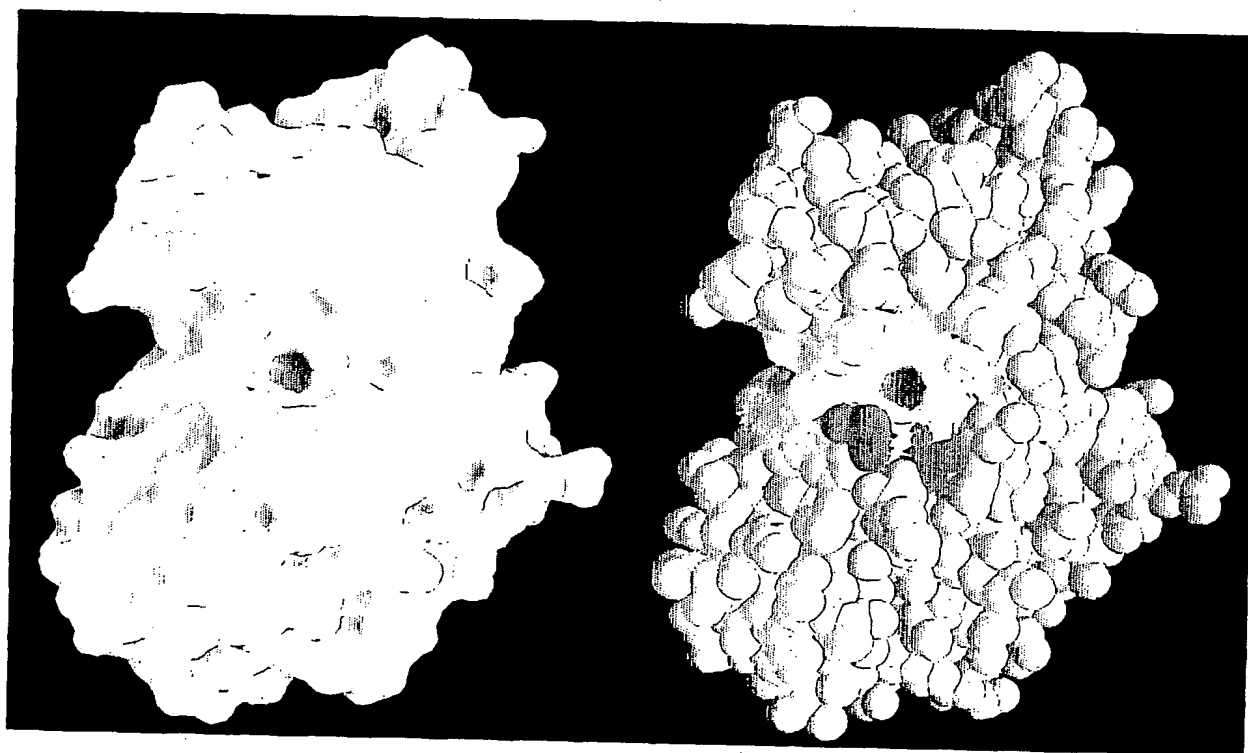


FIG. 18

SUBSTITUTE SHEET (RULE 26)

| | | | | | | | | | | | |
|---------------|--------|-----|---------|-----|---|-----|----|-----|-----|-----|---|
| SEQ ID NO: 30 | hTRβ | 277 | T P A I | 280 | h | 287 | hK | 293 | h F | 309 | h |
| SEQ ID NO: 32 | hTRα | 223 | T P A I | 281 | h | 288 | hK | 293 | h F | 309 | h |
| SEQ ID NO: 34 | hARY | 235 | T K C Q | 282 | h | 289 | hK | 293 | h F | 309 | h |
| SEQ ID NO: 36 | hXRA | 273 | D K C Q | 283 | h | 290 | hK | 293 | h F | 309 | h |
| SEQ ID NO: 38 | hPPARY | 288 | V E A V | 284 | h | 291 | hK | 293 | h F | 309 | h |
| SEQ ID NO: 40 | hVDR | 235 | S Y S I | 285 | h | 292 | hK | 293 | h F | 309 | h |
| SEQ ID NO: 42 | hERα | 351 | D R E L | 286 | h | 293 | hK | 293 | h F | 309 | h |
| SEQ ID NO: 44 | hGR | 568 | G R Q V | 287 | h | 294 | hK | 293 | h F | 309 | h |
| SEQ ID NO: 46 | hPR | 723 | E R Q L | 288 | h | 295 | hK | 293 | h F | 309 | h |
| SEQ ID NO: 48 | hMR | 774 | G K Q M | 289 | h | 296 | hK | 293 | h F | 309 | h |
| SEQ ID NO: 50 | hAR | 242 | E R Q L | 290 | h | 297 | hK | 293 | h F | 309 | h |

| | | | | | | | | | |
|---------------|--------|-----|---------|-----|---|-----|---|-----|---|
| SEQ ID NO: 31 | hTRβ | 450 | L F P P | 453 | h | 458 | h | 459 | h |
| SEQ ID NO: 33 | hTRα | 396 | L F P P | 454 | h | 459 | h | 459 | h |
| SEQ ID NO: 35 | hARY | 407 | P I D P | 455 | h | 460 | h | 461 | h |
| SEQ ID NO: 37 | hXRA | 446 | S L T H | 456 | h | 461 | h | 462 | h |
| SEQ ID NO: 39 | hPPARY | 462 | K L Y D | 457 | h | 462 | h | 463 | h |
| SEQ ID NO: 41 | hVDR | 413 | P L Y D | 458 | h | 463 | h | 464 | h |
| SEQ ID NO: 43 | hERα | 535 | P L Y D | 459 | h | 464 | h | 465 | h |
| SEQ ID NO: 45 | hGR | 748 | E F F P | 460 | h | 465 | h | 466 | h |
| SEQ ID NO: 47 | hPR | 904 | E F F P | 461 | h | 466 | h | 467 | h |
| SEQ ID NO: 49 | hMR | 955 | E F F P | 462 | h | 467 | h | 468 | h |
| SEQ ID NO: 51 | hAR | 423 | D F F P | 463 | h | 468 | h | 469 | h |

FIGURE 19

5 SEQUENCE LISTING

<110> Baxter, John D.
Darimont, Beatrice
Feng, Weijun
10 Fletterick, Robert J.
Kushner, Peter J.
Wagner, Richard L.
West, Brian L.
15 Yamamoto, Keith R.

<120> METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR
COACTIVATOR BINDING

<130> UCAL-253/01US

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1 5

<210> 2

<211> 6

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<213> Homo sapiens

<400> 2

Ile Leu Xaa Xaa Leu Leu

1 5

<210> 3

<211> 5

<212> PRT

<213> Homo sapiens

<400> 3

Phe Xaa Xaa Leu Trp

1 5

<210> 4

<211> 5

<212> PRT

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<400> 4

5 Phe Xaa Xaa Ala Leu
1 5

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1 5 10 15
Leu Gln Leu Leu Thr Thr Lys Ser Glu Gln Met Glu Pro Ser Pro Leu
20 25 30
20 Ala Ser

25 <210> 6
<211> 34
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30 <220>
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35 <220>
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<223> Leu(16) --> Ala; Leu(20) --> Ala

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10 <223> Ile --> Phe

<220>
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<220>
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20 <223> Leu --> Phe

<220>
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<222> (20)

25 <223> Leu --> Phe

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30 His Arg Leu Leu Gln Asp Ser Ser Ser Pro Val Asp Leu Ala Lys Leu
20 25 30

Thr Ala

35

<210> 7
<211> 31
<212> PRT
<213> Homo sapiens

40

<400> 7
Glu Pro Ala Ser Pro Lys Lys Lys Glu Asn Ala Leu Leu Arg Tyr Leu
1 5 10 15

45 Leu Asp Lys Asp Asp Thr Lys Asp Ile Gly Leu Pro Glu Ile Thr
20 25 30

50

<210> 8
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<213> Homo sapiens

55

<400> 8
Ala Asp Gly Gln Ser Arg Leu His Asp Ser Lys Gly Gln Thr Lys Leu
1 5 10 15

60 Leu Gln Leu Leu Thr Thr Lys Ser Glu Gln Met Glu Pro Ser Pro Leu
20 25 30

Ala Ser

65

<210> 9

5 <211> 34
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 <213> Homo sapiens

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 10 Ser Gly Ser Thr His Gly Thr Ser Leu Lys Glu Lys His Lys Ile Leu
 1 5 10 15
 His Arg Leu Leu Gln Asp Ser Ser Ser Pro Val Asp Leu Ala Lys Leu
 20 25 30
 15 Thr Ala

20 <210> 10
 <211> 31
 <212> PRT
 <213> Homo sapiens

25 <400> 10
 Glu Pro Val Ser Pro Lys Lys Lys Glu Asn Ala Leu Leu Arg Tyr Leu
 1 5 10 15
 Leu Asp Lys Asp Asp Thr Lys Asp Ile Gly Leu Pro Glu Ile Thr
 30 20 25 30

<210> 11
 <211> 34
 35 <212> PRT
 <213> Homo sapiens

<400> 11
 40 Ala Glu Gly His Ser Arg Leu His Asp Ser Lys Gly Gln Thr Lys Leu
 1 5 10 15
 Leu Gln Leu Leu Thr Thr Lys Ser Glu Gln Met Glu Pro Ser Pro Leu
 20 25 30
 45 Pro Ser

50 <210> 12
 <211> 34
 <212> PRT
 <213> Homo sapiens

<400> 12
 55 Pro Gly Ser Thr His Gly Thr Ser Leu Lys Glu Lys His Lys Ile Leu
 1 5 10 15
 His Arg Leu Leu Gln Asp Ser Ser Ser Pro Val Asp Leu Ala Lys Leu
 20 25 30
 60 Thr Ala

65 <210> 13
 <211> 31
 <212> PRT

5 <213> Homo sapiens

<400> 13
 Glu Pro Ala Ser Pro Lys Lys Lys Glu Asn Ala Leu Leu Arg Tyr Leu
 1 5 10 15

10 Leu Asp Lys Asp Asp Thr Lys Asp Ile Gly Leu Pro Ser Ile Thr
 20 25 30

15 <210> 14
 <211> 34
 <212> PRT
 <213> Homo sapiens

20 <400> 14
 Ala Glu Asn Gln Arg Gly Pro Leu Glu Ser Lys Gly His Lys Lys Leu
 1 5 10 15

25 Leu Gln Leu Leu Thr Cys Ser Ser Glu Asp Arg Gly His Ser Ser Leu
 20 25 30

Thr Asn

30 <210> 15
 <211> 34
 <212> PRT
 <213> Homo sapiens

35 <400> 15
 Thr Ser Asn Met His Gly Ser Leu Leu Gln Glu Lys His Arg Ile Leu
 1 5 10 15

40 His Lys Leu Leu Gln Asn Gly Asn Ser Pro Ala Glu Val Ala Lys Ile
 20 25 30

Thr Ala

45 <210> 16
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 <212> PRT
 <213> Homo sapiens

50 <400> 16
 Glu Gln Leu Ser Pro Lys Lys Lys Glu Asn Asn Ala Leu Leu Arg Tyr
 1 5 10 15

55 Leu Leu Asp Arg Asp Asp Pro Ser Asp Val Leu Ala Lys Lys Leu Gln
 20 25 30

60 <210> 17
 <211> 34
 <212> PRT
 <213> Homo sapiens

65

5 <400> 17
 Ala Glu Asn Gln Arg Gly Pro Leu Glu Ser Lys Gly His Lys Lys Leu
 1 5 10 15

10 Leu Gln Leu Leu Thr Cys Ser Ser Asp Asp Arg Gly His Ser Ser Leu
 20 25 30

Thr Asn

15 <210> 18
 <211> 34
 <212> PRT
 <213> Homo sapiens

20 <400> 18
 Thr Ser Asn Met His Gly Ser Leu Leu Gln Glu Lys His Arg Ile Leu
 1 5 10 15

25 His Lys Leu Leu Gln Asn Gly Asn Ser Pro Ala Glu Val Ala Lys Ile
 20 25 30

Thr Ala

30 <210> 19
 <211> 32
 <212> PRT
 <213> Homo sapiens

35 <400> 19
 Glu Gln Leu Ser Pro Lys Lys Lys Glu Asn Asn Ala Leu Leu Arg Tyr
 1 5 10 15

40 Leu Leu Asp Arg Asp Asp Pro Ser Asp Ala Leu Ser Lys Glu Leu Gln
 20 25 30

45 <210> 20
 <211> 34
 <212> PRT
 <213> Homo sapiens

50 <400> 20
 Ser Glu Thr Pro Arg Gly Pro Leu Glu Ser Lys Gly His Lys Lys Leu
 1 5 10 15

55 Leu Gln Leu Leu Thr Cys Ser Ser Glu Asp Arg Gly His Ser Ser Leu
 20 25 30

60 Thr Asn

65 <210> 21
 <211> 34
 <212> PRT
 <213> Homo sapiens

5

<400> 21

Thr Ser Asn Val His Gly Ser Leu Leu Gln Glu Lys His Arg Ile Leu
 1 5 10 15

10 His Lys Leu Leu Gln Asn Gly Asn Ser Pro Ala Glu Val Ala Lys Ile
 20 25 30

Thr Ala

15

<210> 22

<211> 32

<212> PRT

20 <213> Homo sapiens

<400> 22

Glu Gln Leu Ser Pro Lys Lys Lys Glu Asn Asn Ala Leu Leu Arg Tyr
 1 5 10 15

25 Leu Leu Asp Arg Asp Asp Pro Ser Asp Ala Leu Ser Lys Glu Leu Gln
 20 25 30

30

<210> 23

<211> 32

35 <212> PRT

<213> Homo sapiens

<400> 23

40 Ser Glu Gly Asp Ser Lys Tyr Ser Gln Thr Ser His Lys Leu Val Gln
 1 5 10 15

Leu Leu Thr Thr Thr Ala Glu Gln Gln Leu Arg His Ala Asp Ile Asp
 20 25 30

45

<210> 24

50 <211> 33

<212> PRT

<213> Homo sapiens

<400> 24

55 Thr Cys Pro Ser Ser His Ser Ser Leu Thr Glu Arg His Lys Ile Leu
 1 5 10 15

His Arg Leu Leu Gln Glu Gly Ser Pro Ser Asp Ile Thr Thr Leu Ser
 20 25 30

60

Val

65

<210> 25

<211> 34

<212> PRT

5 <213> Homo sapiens

<400> 25

Glu Leu Asp Ala Ala Lys Lys Lys Glu Ser Lys Asp His Gln Leu Leu
1 5 10 15

10 Arg Tyr Leu Leu Asp Lys Asp Glu Lys Asp Leu Arg Ser Thr Pro Asn
20 25 30

Leu Cys

15

<210> 26

<211> 34

20 <212> PRT

<213> Homo sapiens

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25 <222> (2)

<223> negatively charged amino acid

<220>

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30 <222> (17)

<223> hydrophobic amino acid

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35 <222> (25)

<223> negatively charged amino acid

<400> 26

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1 5 10 15

Xaa Gln Leu Leu Thr Xaa Xaa Xaa Xaa Xaa Xaa Xaa Xaa Xaa Xaa
20 25 30

45 Xaa Xaa

<210> 27

50 <211> 34

<212> PRT

<213> Homo sapiens

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55 <221> SITE

<222> (12)

<223> positively charged amino acid

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60 <221> SITE

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<220>

65 <221> SITE

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5

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10

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```

15

```
<220>  
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<222> (32)  
<223> hydrophobic amino acid
```

20

<400> 27
Xaa Xaa Xaa Xaa Xaa Xaa Xaa Xaa Leu Xaa Glu Xaa His Xaa Ile Leu
1 5 10 15

25 His Xaa Leu Leu Gln Xaa Xaa Xaa Ser Pro Xaa Xaa Xaa Xaa Xaa Xaa
20 25 30

Xaa Xaa

30

```
<210> 28
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35

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<220>
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45

```
<220>  
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<222> (33)  
<223> hydrophobic amino acid
```

50

<400> 28
Glu Xaa Xaa Xaa Xaa Lys Lys Lys Glu Xaa Xaa Xaa Xaa Xaa Leu Leu
1 5 10 15

55

Arg Tyr Leu Leu Asp Xaa Asp Xaa Xaa Xaa Xaa Xaa Xaa Xaa Xaa Xaa Xaa
20 25 30

Xaa Xaa

60

```
<210> 29
<211> 18
<212> PRT
<213> Homo sapiens
```

65

5 <400> 29
 Thr Ser Leu Lys Glu Lys His Lys Leu Leu Arg Tyr Leu Leu Gln Asp
 1 5 10 15

10 Ser Ser

15 <210> 30
 <211> 33
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20 <220>
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 <222> (5)
 <223> Thr --> Arg (T281R)

25 <220>
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 <222> (8)
 <223> Val --> Arg (V284R)

30 <220>
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 <223> Asp --> Ala (D285A)

35 <220>
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 <223> Lys --> Ala (K288A)

40 <220>
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45 <220>
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 <222> (26)
 <223> Ile --> Arg (I302R)

50 <220>
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 <222> (30)
 <223> Lys --> Ala (K306A)

55 <400> 30
 Thr Pro Ala Ile Thr Arg Val Val Asp Phe Ala Lys Lys Leu Pro Met
 1 5 10 15

Phe Cys Glu Leu Pro Cys Glu Asp Gln Ile Ile Leu Leu Lys Gly Cys
 20 25 30

60 Cys

65 <210> 31
 <211> 12
 <212> PRT
 <213> Homo sapiens

5

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<222> (5)
<223> Leu --> Arg (L454R)

10

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<222> (7)
<223> Leu --> Arg (L456R)

15

<220>
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<222> (8)
<223> Glu --> Lys (E457K)

20

<400> 31
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1 5 10

25

<210> 32
<211> 33
<212> PRT
<213> Homo sapiens

30

<400> 32
Thr Pro Ala Ile Thr Arg Val Val Asp Phe Ala Lys Lys Leu Pro Met
1 5 10 15

35

Phe Ser Glu Leu Pro Cys Glu Asp Gln Ile Ile Leu Leu Lys Gly Cys
20 25 30

Cys

40

<210> 33
<211> 12
<212> PRT
<213> Homo sapiens

45

<400> 33
Leu Phe Pro Pro Leu Phe Leu Glu Val Phe Glu Asp
1 5 10

50

<210> 34
<211> 33
<212> PRT
<213> Homo sapiens

55

<400> 34
Thr Lys Cys Ile Ile Lys Ile Val Glu Phe Ala Lys Arg Leu Pro Gly
1 5 10 15

60

Phe Thr Gly Leu Ser Ile Ala Asp Gln Ile Thr Leu Leu Lys Ala Ala
20 25 30

Cys

65

5 <210> 35
 <211> 12
 <212> PRT
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10 <400> 35
 Leu Phe Pro Pro Leu Phe Leu Glu Val Phe Glu Asp
 1 5 10

15 <210> 36
 <211> 33
 <212> PRT
 <213> Homo sapiens

20 <400> 36
 Asp Lys Gln Leu Phe Thr Leu Val Glu Trp Ala Lys Arg Ile Pro His
 1 5 10 15

25 Phe Ser Glu Leu Pro Leu Asp Asp Gln Val Ile Leu Leu Lys Ala Gly
 20 25 30

Trp

30 <210> 37
 <211> 12
 <212> PRT
 <213> Homo sapiens

35 <400> 37
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 1 5 10

40 <210> 38
 <211> 33
 <212> PRT
 <213> Homo sapiens

45 <400> 38
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 1 5 10 15

50 Phe Ile Asn Leu Asp Leu Asn Asp Gln Val Thr Leu Leu Lys Tyr Gly
 20 25 30

Val

55 <210> 39
 <211> 12
 <212> PRT
 <213> Homo sapiens

60 <400> 39
 Ser Leu His Pro Leu Leu Gln Glu Ile Tyr Lys Asp
 1 5 10

65 <210> 40

5 <211> 33
 <212> PRT
 <213> Homo sapiens

10 <400> 40
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 1 5 10 15
 Phe Arg Asp Leu Thr Ser Glu Asp Gln Ile Val Leu Leu Lys Ser Ser
 20 25 30
 15 Ala

20 <210> 41
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 <212> PRT
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25 <400> 41
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 1 5 10

30 <210> 42
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 20 25 30
 50 Trp

55 <210> 43
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 <213> Homo sapiens

60 <220>
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5 1 5 10

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 1 5 10 15

 Phe Arg Asn Leu His Leu Asp Asp Gln Met Thr Leu Leu Gln Tyr Ser
 20 25 30

20 Trp

25 <210> 45
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30 <400> 45
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 1 5 10

35 <210> 46
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 Phe Arg Asn Leu His Ile Asp Asp Gln Ile Thr Leu Ile Gln Tyr Ser
 20 25 30

45 Trp

50 <210> 47
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 1 5 10

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 Gly Lys Gln Met Ile Gln Val Val Lys Trp Ala Lys Val Leu Pro Gly
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Phe Lys Asn Leu Pro Leu Glu Asp Gln Ile Thr Leu Ile Gln Tyr Ser
 20 25 30

10

Trp

15

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20

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Glu Phe Pro Ala Met Leu Val Glu Ile Ile Ser Asp
 1 5 10

25

<210> 50

<211> 33

<212> PRT

<213> Homo sapiens

30

<400> 50

Glu Arg Gln Leu Val His Val Val Lys Trp Ala Lys Ala Leu Pro Gly
 1 5 10 15

Phe Arg Asn Leu His Val Asp Asp Gln Met Ala Val Ile Gln Tyr Ser
 20 25 30

35

Trp

40

<210> 51

<211> 12

<212> PRT

<213> Homo sapiens

45

<400> 51

Asp Phe Pro Glu Met Met Ala Glu Ile Ile Ser Val
 1 5 10

50

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US99/06899

A. CLASSIFICATION OF SUBJECT MATTER

IPC(7) :G01N 33/50

US CL :435/7.1

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

U.S. : 435/7.1

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

Please See Extra Sheet.

C. DOCUMENTS CONSIDERED TO BE RELEVANT

| Category* | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No. |
|-----------------|---|-----------------------|
| X ----- A | WAGNER et al. A structural role for hormone in the thyroid hormone receptor. Nature. 14 December 1995, Vol. 378, pages 690-697, especially page 690 and figure 1 and 2 and Table 1. | 1 ----- 2-30 |

☐ Further documents are listed in the continuation of Box C.☐ See patent family annex.

| | |
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| *P* document published prior to the international filing date but later than the priority date claimed | |

Date of the actual completion of the international search

01 DECEMBER 1999

Date of mailing of the international search report

29 FEB 2000

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INTERNATIONAL SEARCH REPORT

International application No.

PCT/US99/06899

Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)

This international report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:
2. ☐ Claims Nos.:
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:
3. ☐ Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

Please See Extra Sheet.

1. ☒ As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.
2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. ☐ As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:
4. ☐ No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

☐
☐

The additional search fees were accompanied by the applicant's protest.

No protest accompanied the payment of additional search fees.

Form PCT/ISA/210 (continuation of first sheet(1))(July 1992)★

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